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 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  FEB 28   PATDPAFULL - New display fields provide for legal status
                   data from INPADOC
 NEWS  4  FEB 28   BABS - Current-awareness alerts (SDIs) available
 NEWS  5  MAR 02   GBFULL: New full-text patent database on STN
 NEWS  6  MAR 03   REGISTRY/ZREGISTRY - Sequence annotations enhanced
 NEWS  7  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS  8  MAR 22   KOREAPAT now updated monthly; patent information enhanced
 NEWS  9  MAR 22   Original IDE display format returns to REGISTRY/ZREGISTRY
 NEWS  10 MAR 22   PATDPASPC - New patent database available
 NEWS  11 MAR 22   REGISTRY/ZREGISTRY enhanced with experimental property tags
 NEWS  12 APR 04   EPFULL enhanced with additional patent information and new
                   fields
 NEWS  13 APR 04   EMBASE - Database reloaded and enhanced
 NEWS  14 APR 18   New CAS Information Use Policies available online
 NEWS  15 APR 25   Patent searching, including current-awareness alerts (SDIs),
                   based on application date in CA/CAplus and USPATFULL/USPAT2
                   may be affected by a change in filing date for U.S.
                   applications.
 NEWS  16 APR 28   Improved searching of U.S. Patent Classifications for
                   U.S. patent records in CA/CAplus
 NEWS  17 MAY 23   GBFULL enhanced with patent drawing images
 NEWS  18 MAY 23   REGISTRY has been enhanced with source information from
                   CHEMCATS
 NEWS  19 JUN 06   STN Patent Forums to be held in June 2005
 NEWS  20 JUN 06   The Analysis Edition of STN Express with Discover!
                   (Version 8.0 for Windows) now available
 NEWS  21 JUN 13   RUSSIAPAT: New full-text patent database on STN
 NEWS  22 JUN 13   FRFULL enhanced with patent drawing images
 NEWS  23 JUN 20   MEDICONF to be removed from STN

 NEWS EXPRESS  JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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FILE 'HOME' ENTERED AT 13:37:49 ON 26 JUN 2005

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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DICTIONARY FILE UPDATES: 24 JUN 2005 HIGHEST RN 852980-90-6

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****
* *
* The CA roles and document type information have been removed from *
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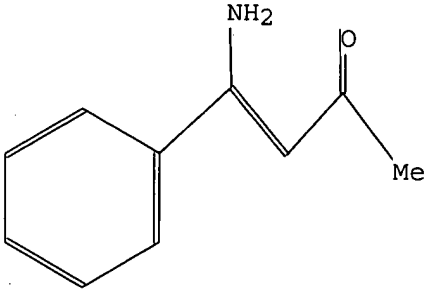
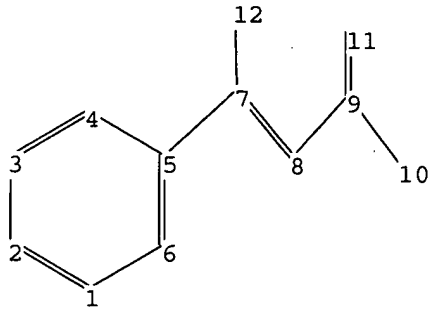
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10658754.str





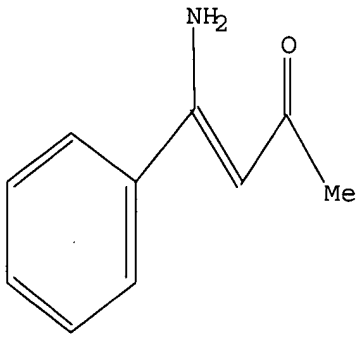
chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6

chain bonds :
5-7 7-8 7-12 8-9 9-10 9-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-12 9-11
exact bonds :
5-7 7-8 8-9 9-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 13:38:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   3592 TO ITERATE

100.0% PROCESSED   3592 ITERATIONS   59 ANSWERS
SEARCH TIME: 00.00.01

L2   59 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                        ENTRY   SESSION
FULL ESTIMATED COST   161.33   161.54

FILE 'CAPLUS' ENTERED AT 13:38:57 ON 26 JUN 2005
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FILE COVERS 1907 - 26 Jun 2005 VOL 143 ISS 1
FILE LAST UPDATED: 24 Jun 2005 (20050624/ED)

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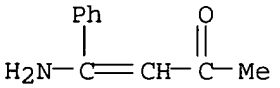
This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l2
L3          47 L2

=> s l3 and (formaldehyde)
        135314 FORMALDEHYDE
           371 FORMALDEHYDES
        135419 FORMALDEHYDE
                  (FORMALDEHYDE OR FORMALDEHYDES)
L4           3 L3 AND (FORMALDEHYDE)

=> d l4 hitstr, ibib, iabs
```

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of detection reagent for color-production-type indoor-air **formaldehyde** detectors)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2004:451033 CAPLUS
DOCUMENT NUMBER: 140:427959
TITLE: Color-production-type indoor-air **formaldehyde** detectors
INVENTOR(S): Nakano, Nobuo; Kawabe, Tetsuya; Terauchi, Yasuhiro; Suzuki, Koji
PATENT ASSIGNEE(S): Riken Keiki Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

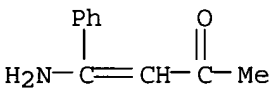
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004157103	A2	20040603	JP 2003-58197	20030305
US 2004197225	A1	20041007	US 2003-658754	20030910

PRIORITY APPLN. INFO.: JP 2002-263713 A 20020910
ABSTRACT:
Silica gel-containing planar substrates are impregnated with color-producing solns. containing 4-amino-4-phenyl-3-en-2-one compds. and buffer solns. and then subjected

to vaporizing solvents to give the **formaldehyde** detectors. The detectors show high sensitivity and quick response.

=> d l4 hitstr, ibib, iabs 2, 3

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(colorimetric reagents for determination of **formaldehyde** in air)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



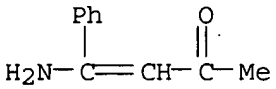
ACCESSION NUMBER: 2003:884712 CAPLUS
DOCUMENT NUMBER: 140:63776
TITLE: Portable Sick House Syndrome Gas Monitoring System Based on Novel Colorimetric Reagents for the Highly Selective and Sensitive Detection of **Formaldehyde**
AUTHOR(S): Suzuki, Yoshio; Nakano, Nobuo; Suzuki, Koji
CORPORATE SOURCE: Regional Entities for the Advancement of Technological Excellence (CREATE), Kanagawa Academy of Science and Technology, Kawasaki, Kanagawa, 213-0012, Japan
SOURCE: Environmental Science and Technology (2003), 37(24), 5695-5700
CODEN: ESTHAG; ISSN: 0013-936X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:

Formaldehyde (HCHO) emitted from the furniture and the walls in the rooms injures the eyes, nose, and respiratory organs and causes allergies, which is called sick house syndrome. We designed and synthesized novel colorimetric HCHO-sensing mols. (KD-XA01 and KD-XA02) which possess an enaminone structure and developed a hand-held instrument to monitor indoor HCHO gas with the use of KD-XA01. These sensing mols. produced speedy color changes from colorless to yellow under mild conditions, which was caused by the fact that the enaminone structure in the reagent reacts with HCHO to give a lutidine derivative This reaction took place not only in the solution phase but also in the solid phase (surface of the cellulose paper). To take advantage of this phenomena, a handy and rapid monitoring system has been developed for detecting indoor HCHO gas using a highly sensitive and selective detection tablet constructed from the porous cellulose paper that contains silica gel as an adsorbent, KD-XA01, and phosphoric acid under optimum conditions. This instrument detected the surface color change of the tablet from white to yellow, which was monitored as a function of the intensity of the reflected light illuminated by an LED (475 nm). The response was proportional to the HCHO concentration at a constant sampling time and flow rate; 0.05 ppm HCHO, which is under the standard value set by the World Health Organization, was able to be detected in 5 min. The detection limit was 0.005 ppm. This monitoring system was not interfered by carbonyl compds. such as acetaldehyde and acetone, alcs., hydrocarbons, and typical gases such as carbon monoxide, carbon dioxide, nitrogen dioxide, etc., which contributes to the measurement of correct HCHO concns. It was possible to monitor the HCHO gas in the room of a new apartment and school using this instrument; the response values were in good agreement with those obtained by the standard DNPH method. This highly sensitive, selective,

and handy HCHO gas monitor is widely applicable and convenient for users who are not specialists in this field.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P**
RL: ARG (Analytical reagent use); IMF (Industrial manufacture); ANST (Analytical study); PREP (Preparation); USES (Uses)
(aromatic amine anal. reagent for detection or determination of **formaldehyde** in indoor air)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



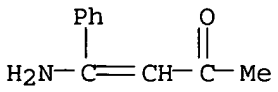
ACCESSION NUMBER: 2003:568771 CAPLUS
DOCUMENT NUMBER: 139:127084
TITLE: Analytical reagent and its use in method for detection or determination of **formaldehyde**
INVENTOR(S): Suzuki, Koji; Suzuki, Sachio
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan; Kanagawa Academy of Science and Technology
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003207498	A2	20030725	JP 2002-7885	20020116

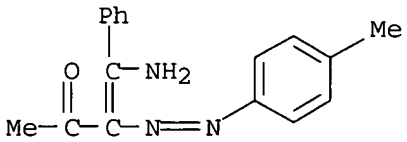
PRIORITY APPLN. INFO.: JP 2002-7885 20020116
OTHER SOURCE(S): MARPAT 139:127084
ABSTRACT:
The reagent contains R22NC(Ar):CHC(O)R1 [R1 = H, C1-10 linear or branched alkyl, (un)substituted Ph; R2 = H, C1-10 linear or branched alkyl; Ar = (un)substituted Ph, naphthyl, anthracenyl]. The above compound may be fixed on filter paper. HCHO is measured by bringing the agent into contact with a sample and detecting or determining the formed colorant. The agent is suitable for HCHO anal. in indoor air.

=> d l3 hitstr, ibib, iabs 1-47

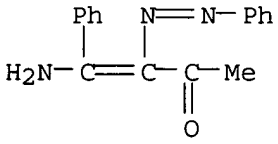
L3 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(azo coupling; solution and solid state structure and tautomerism of azo coupled enaminone derivs. of benzoylacetone)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



IT **849926-45-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; solution and solid state structure and tautomerism of azo coupled enaminone derivs. of benzoylacetone)
RN 849926-45-0 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[(4-methylphenyl)azo]-4-phenyl- (9CI) (CA INDEX NAME)



IT **849926-46-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(solution and solid state structure and tautomerism of azo coupled enaminone derivs. of benzoylacetone)
RN 849926-46-1 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-3-(phenylazo)- (9CI) (CA INDEX NAME)



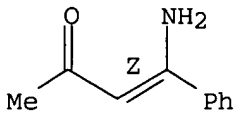
ACCESSION NUMBER: 2005:246001 CAPLUS
DOCUMENT NUMBER: 142:392052
TITLE: Solution and solid state structure and tautomerism of azo coupled enaminone derivatives of benzoylacetone
AUTHOR(S): Simunek, Petr; Bertolasi, Valerio; Peskova, Marketa; Machacek, Vladimir; Lycka, Antonin
CORPORATE SOURCE: University of Pardubice, Pardubice, CZ-532 10, Czech Rep.
SOURCE: Organic & Biomolecular Chemistry (2005), 3(7), 1217-1226
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The reaction of 4-substituted benzenediazonium tetrafluoroborates with 3-amino-1-phenylbut-2-en-1-one, 4-amino-4-phenylbut-3-en-2-one and their N-aryl derivs. has been used to prepare the resp. azo coupling products. Tautomerism of the azo coupling products prepared has been investigated in CDCl3 solns. by means of 1H, 13C and 15N NMR spectra. Crystal structures of selected products have also been investigated by means of X-ray diffraction.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **95514-24-2P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(reaction of 3-phenylisoxazole with alkyllithiums)
RN 95514-24-2 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

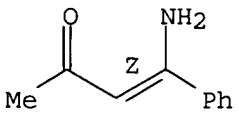


ACCESSION NUMBER: 2005:162254 CAPLUS
DOCUMENT NUMBER: 142:391962
TITLE: Reaction of 3-phenylisoxazole with alkyllithiums
AUTHOR(S): Di Nunno, Leonardo; Scilimati, Antonio; Vitale, Paola
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy
SOURCE: Tetrahedron (2005), 61(10), 2623-2630
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Alkyllithiums react with 3-phenylisoxazole giving C5-H abstraction followed either mainly by ring fragmentation to benzonitrile and ethynolate ion (in the case of t-BuLi) or (less hindered alkyllithiums: n-BuLi, EtLi, MeLi) also by formation of alkylated enaminones. Appreciable amts. of 2-alkyl-4,6-diphenylpyrimidines have also been isolated for certain alkyllithiums (EtLi and MeLi). This is at variance with the reported behavior with hindered lithium amides (LTMP) for which only C5-H abstraction followed by ring fragmentation was described. The mechanistic significance of the observed results is discussed.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

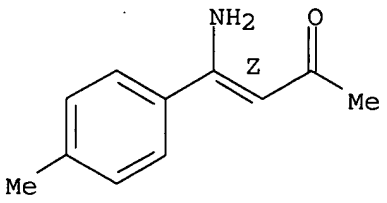
L3 ANSWER 3 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **95514-24-2P 798555-51-8P 798555-72-3P**
798555-73-4P 798555-74-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of (isoxazolyl)(hydroxy) esters, enaminones, pyridones and dihydrofuranones via catalytic hydrogenation of Baylis-Hillman adducts of isoxazolecarboxaldehydes or their acetates)
RN 95514-24-2 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



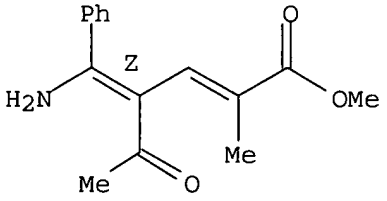
RN 798555-51-8 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-methylphenyl)-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



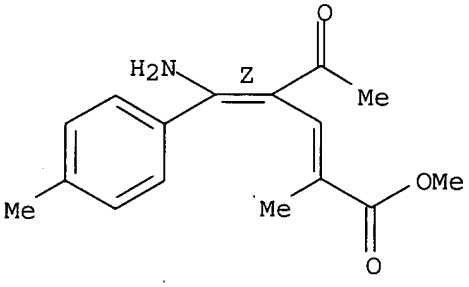
RN 798555-72-3 CAPLUS
CN 2-Hexenoic acid, 4-(aminophenylmethylene)-2-methyl-5-oxo-, methyl ester, (4Z)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.



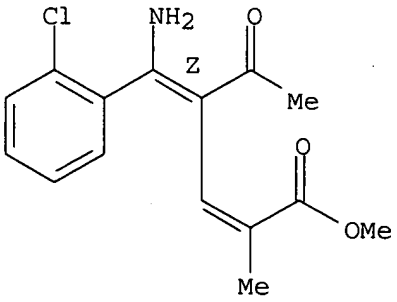
RN 798555-73-4 CAPLUS
CN 2-Hexenoic acid, 4-[amino(4-methylphenyl)methylene]-2-methyl-5-oxo-, methyl ester, (4Z)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.



RN 798555-74-5 CAPLUS
CN 2-Hexenoic acid, 4-[amino(2-chlorophenyl)methylene]-2-methyl-5-oxo-, methyl ester, (4Z)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.



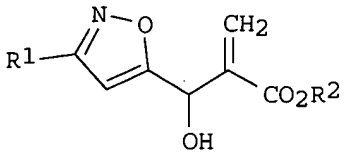
ACCESSION NUMBER: 2004:815667 CAPLUS
DOCUMENT NUMBER: 142:6460
TITLE: Studies on the catalytic hydrogenation of

Baylis-Hillman derivatives of substituted isoxazolecarbaldehydes. Unusual retention of isoxazole ring during Pd-C-promoted hydrogenation of Baylis-Hillman adducts

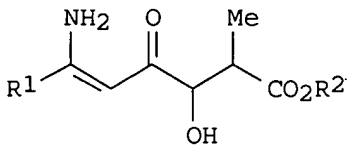
AUTHOR(S): Saxena, R.; Singh, V.; Batra, S.
CORPORATE SOURCE: Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, 226 001, India

SOURCE: Tetrahedron (2004), 60(45), 10311-10320
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6460

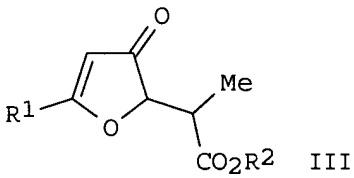
GRAPHIC IMAGE:



I



II

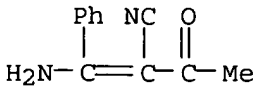


III

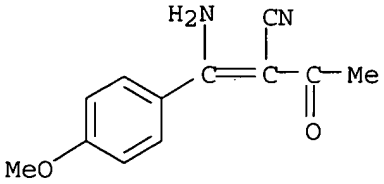
ABSTRACT:
Results of the catalytic hydrogenation of Baylis-Hillman adducts obtained from substituted 3-, 4- and 5-isoxazolecarboxaldehydes, e.g. I (R1 = Ph, 4-MeC6H4, 2-ClC6H4, 4-ClC6H4; R2 = Me, Et), and their acetates in the presence of Raney-Ni and Pd-C are presented. The hydrogenation of Baylis-Hillman adducts of substituted 5-isoxazolecarboxaldehydes and 3-isoxazolecarboxaldehydes in the presence of Raney-Ni furnishes diastereoselectively enaminones, e.g. II from I, favoring the syn diastereomer over the anti and in the presence of boric acid as an additive further enhancement of diastereoselectivity in favor of syn isomer is observed The Pd-C-promoted hydrogenation of these substrates is also diastereoselective in favor of syn isomer but occurs without the hydrogenolysis of isoxazole-ring. The presence of boric acid as an additive in this hydrogenation exhibits no pronounced effect on diastereoselectivity. The Raney-Ni-mediated hydrogenation of Baylis-Hillman adducts of substituted 4-isoxazolecarboxaldehydes yield pyridone derivs. and Pd-C-promoted hydrogenation of the same substrate is diastereoselective to afford the anti isomers. The enaminones derived from Baylis-Hillman adducts of 3- and 5-isoxazolecarboxaldehydes serve as versatile precursors for α'-hydroxy-1,3-diketones, which undergo acid-catalyzed ring-closure reaction to afford the furanone derivs., e.g. III, in excellent yields.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **33831-49-1 756531-37-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3,5-disubstituted-4-isothiazolecarbonitriles starting from α-cyano-β-enaminones via oxidative cyclization of thiones)
RN 33831-49-1 CAPLUS
CN Butanenitrile, 2-(aminophenylmethylene)-3-oxo- (9CI) (CA INDEX NAME)



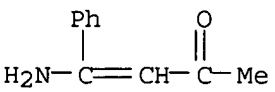
RN 756531-37-0 CAPLUS
CN Butanenitrile, 2-[amino(4-methoxyphenyl)methylene]-3-oxo- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2004:574585 CAPLUS
DOCUMENT NUMBER: 141:260612
TITLE: Synthesis of novel 3,5-disubstituted-4-isothiazolecarbonitriles
AUTHOR(S): Mishra, Manisha; Dutta Chowdhury, S. K.; Mahalanabis, Kumar K.
CORPORATE SOURCE: Department of Chemistry, Jadavpur University, Kolkata, India
SOURCE: Synthetic Communications (2004), 34(14), 2681-2689
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:260612
ABSTRACT:
α-Cyano-β-enaminones, obtained by regioselective acylation of β-enaminonitriles, were smoothly converted to thiones which on oxidative cyclization afforded 3,5-disubstituted-4-isothiazolecarbonitriles in good to excellent yields.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of detection reagent for color-production-type indoor-air formaldehyde detectors)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2004:451033 CAPLUS
DOCUMENT NUMBER: 140:427959
TITLE: Color-production-type indoor-air formaldehyde detectors
INVENTOR(S): Nakano, Nobuo; Kawabe, Tetsuya; Terauchi, Yasuhiro; Suzuki, Koji
PATENT ASSIGNEE(S): Riken Keiki Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

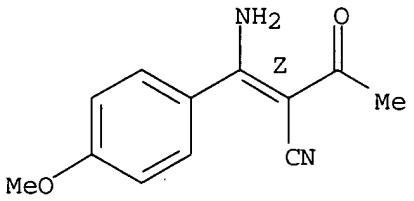
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2004157103	A2	20040603	JP 2003-58197		20030305
US 2004197225	A1	20041007	US 2003-658754		20030910
PRIORITY APPLN. INFO.:			JP 2002-263713	A	20020910

ABSTRACT:
Silica gel-containing planar substrates are impregnated with color-producing solns. containing 4-amino-4-phenyl-3-en-2-one compds. and buffer solns. and then subjected to vaporizing solvents to give the formaldehyde detectors. The detectors show high sensitivity and quick response.

L3 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **698366-92-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazoles by regiospecific cyclocondensation of α-cyano-β-enaminones with phenylhydrazine)
RN 698366-92-6 CAPLUS
CN Butanenitrile, 2-[amino(4-methoxyphenyl)methylene]-3-oxo-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



ACCESSION NUMBER: 2004:265911 CAPLUS
DOCUMENT NUMBER: 141:23468
TITLE: A short and expeditious regiospecific synthesis of novel pyrazoles
AUTHOR(S): Dutta Chowdhury, S. K.; Sarkar, Mili; Mahalanabis, Kumar K.
CORPORATE SOURCE: Jogesh Chandra Choudhuri College, Kolkata, 700 033, India
SOURCE: Journal of Chemical Research, Synopses (2003), (11), 746-748
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Science Reviews
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:23468

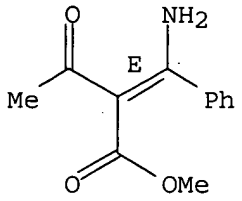
ABSTRACT:
α-Cyano-β-enaminones, obtained by regioselective acylation of β-aminocrotononitrile, are smoothly and regiospecifically converted into substituted pyrazoles in good to excellent yields.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **654061-92-4P**
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)

(stereoselective preparation of arylacylaminoacrylates)
RN 654061-92-4 CAPLUS
CN Butanoic acid, 2-(aminophenylmethylene)-3-oxo-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



ACCESSION NUMBER: 2004:101118 CAPLUS
DOCUMENT NUMBER: 140:163584
TITLE: Preparation of (E)-β-aryl-β-acylaminoacrylates
INVENTOR(S): Heller, Detlef; Drexler, Hans-Joachim; You, Jingsong; Zhang, Songlin
PATENT ASSIGNEE(S): DSM Ip Assets B.V., Neth.
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

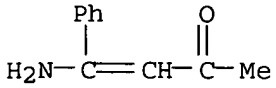
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011414	A1	20040205	WO 2003-NL544	20030725

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2002-10235916 A 20020726
OTHER SOURCE(S): CASREACT 140:163584; MARPAT 140:163584
ABSTRACT:
R2CONR3CR1C:CHCO2R [R, R2 = H, (substituted) alkyl, aryl, heteroaryl; R1 = (substituted) aryl, heteroaryl; R3 = H, (substituted) alkyl, acyl, aryl, heteroaryl], were prepared Thus, 3-amino-3-phenylacrylic acid Me ester and pyridine in THF at -78° were treated with AcCl; within 30 min, the reaction mixture was heated to 0° and stirred for further 8 h. It was stirred for 16 h at room temperature, cooled to 0°, treated with AcCl, and stirred for a further 8 h to give 20.2% pure Me (E)-3-acetamido-3-phenyl-2-propenoate after recrystn.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(colorimetric reagents for determination of formaldehyde in air)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)

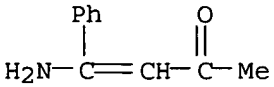


ACCESSION NUMBER: 2003:884712 CAPLUS
DOCUMENT NUMBER: 140:63776
TITLE: Portable Sick House Syndrome Gas Monitoring System Based on Novel Colorimetric Reagents for the Highly Selective and Sensitive Detection of Formaldehyde
AUTHOR(S): Suzuki, Yoshio; Nakano, Nobuo; Suzuki, Koji
CORPORATE SOURCE: Regional Entities for the Advancement of Technological Excellence (CREATE), Kanagawa Academy of Science and Technology, Kawasaki, Kanagawa, 213-0012, Japan
SOURCE: Environmental Science and Technology (2003), 37(24), 5695-5700
CODEN: ESTHAG; ISSN: 0013-936X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:

Formaldehyde (HCHO) emitted from the furniture and the walls in the rooms injures the eyes, nose, and respiratory organs and causes allergies, which is called sick house syndrome. We designed and synthesized novel colorimetric HCHO-sensing mols. (KD-XA01 and KD-XA02) which possess an enaminone structure and developed a hand-held instrument to monitor indoor HCHO gas with the use of KD-XA01. These sensing mols. produced speedy color changes from colorless to yellow under mild conditions, which was caused by the fact that the enaminone structure in the reagent reacts with HCHO to give a lutidine derivative This reaction took place not only in the solution phase but also in the solid phase (surface of the cellulose paper). To take advantage of this phenomena, a handy and rapid monitoring system has been developed for detecting indoor HCHO gas using a highly sensitive and selective detection tablet constructed from the porous cellulose paper that contains silica gel as an adsorbent, KD-XA01, and phosphoric acid under optimum conditions. This instrument detected the surface color change of the tablet from white to yellow, which was monitored as a function of the intensity of the reflected light illuminated by an LED (475 nm). The response was proportional to the HCHO concentration at a constant sampling time and flow rate; 0.05 ppm HCHO, which is under the standard value set by the World Health Organization, was able to be detected in 5 min. The detection limit was 0.005 ppm. This monitoring system was not interfered by carbonyl compds. such as acetaldehyde and acetone, alcs., hydrocarbons, and typical gases such as carbon monoxide, carbon dioxide, nitrogen dioxide, etc., which contributes to the measurement of correct HCHO concns. It was possible to monitor the HCHO gas in the room of a new apartment and school using this instrument; the response values were in good agreement with those obtained by the standard DNPH method. This highly sensitive, selective, and handy HCHO gas monitor is widely applicable and convenient for users who are not specialists in this field.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 47 CAPLUS
IT **14088-41-6P**
RL: ARG (Analytical reagent use); IMF (Industrial manufacture); ANST (Analytical study); PREP (Preparation); USES (Uses)
(aromatic amine anal. reagent for detection or determination of formaldehyde in indoor air)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)

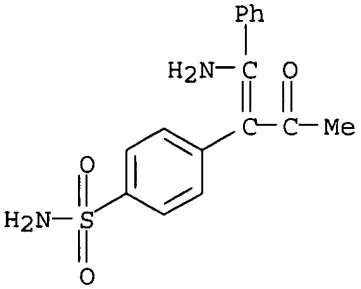


ACCESSION NUMBER: 2003:568771 CAPLUS
DOCUMENT NUMBER: 139:127084
TITLE: Analytical reagent and its use in method for detection or determination of formaldehyde
INVENTOR(S): Suzuki, Koji; Suzuki, Sachio
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan; Kanagawa Academy of Science and Technology
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003207498	A2	20030725	JP 2002-7885	20020116
PRIORITY APPLN. INFO.:			JP 2002-7885	20020116

OTHER SOURCE(S): MARPAT 139:127084
ABSTRACT:
The reagent contains R22NC(Ar):CHC(O)R1 [R1 = H, C1-10 linear or branched alkyl, (un)substituted Ph; R2 = H, C1-10 linear or branched alkyl; Ar = (un)substituted Ph, naphthyl, anthracenyl]. The above compound may be fixed on filter paper. HCHO is measured by bringing the agent into contact with a sample and detecting or determining the formed colorant. The agent is suitable for HCHO anal. in indoor air.

L3 ANSWER 10 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **603151-45-7**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(pharmacokinetics and metabolism of valdecoxib in mice)
RN 603151-45-7 CAPLUS
CN Benzenesulfonamide, 4-[1-(aminophenylmethylene)-2-oxopropyl]- (9CI) (CA INDEX NAME)



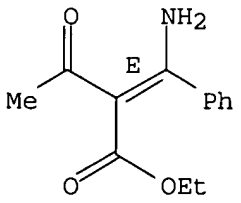
ACCESSION NUMBER: 2003:253158 CAPLUS
DOCUMENT NUMBER: 139:254694
TITLE: Pharmacokinetics and metabolism of a COX-2 inhibitor, valdecoxib, in mice
AUTHOR(S): Zhang, Ji Y.; Yuan, Josh J.; Wang, Yue-Fen; Bible, Roy H., Jr.; Breau, Alan P.
CORPORATE SOURCE: Global Drug Metabolism, Pharmacia, Skokie, IL, 60077, USA

SOURCE: Drug Metabolism and Disposition (2003), 31(4), 491-501
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The pharmacokinetics and metabolism of valdecoxib, a potent cyclooxygenase-2 selective inhibitor, were investigated in mice. Valdecoxib was extensively metabolized after a single 5 mg/kg oral administration of [14C]valdecoxib and elimination of unchanged drug was minor (less than 1%) in male and female mice. The total mean percentage of administered radioactive dose recovered was 99.8% in the male mice and 94.7% in the female mice. Sixteen metabolites were identified in mouse plasma, red blood cells, urine, and feces. The main phase I metabolic pathway of valdecoxib in mice involved the oxidation of the 5-Me group to form the active hydroxymethyl metabolite M1. M1 was further oxidized to the carboxylic acid metabolite M4, which underwent opening of the isoxazole ring to form M6 and M13. Phase II metabolism included glucuronide, glucoside, and Me sulfone conjugations. M1 was also conjugated with glucuronic acid and glucose to yield M-G and M1-glucose, resp. Three novel methylsulfone conjugates M20, M21, and M21-G were detected in blood or urine. Valdecoxib and M1 were the major radioactive components in plasma and red blood cells. The plasma area under the curve from zero to infinity (AUC0-∞) values for valdecoxib and M1 were 3.58 and 0.850 μg·h/mL in males and 2.08 and 1.63 μg·h/mL in females, resp. The RBC AUC0-∞ values for valdecoxib and M1 were 12.1 and 22.6 μg·h/g in males and 6.42 and 35.2 μg·h/g in females, resp.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **495417-87-3**, Ethyl (E)-2-acetyl-3-amino-3-phenyl-2-propylenoate
RL: PRP (Properties)
(crystal structure of)
RN 495417-87-3 CAPLUS
CN Butanoic acid, 2-(aminophenylmethylene)-3-oxo-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

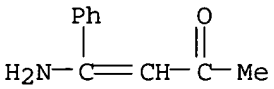


ACCESSION NUMBER: 2002:911881 CAPLUS
DOCUMENT NUMBER: 138:161351
TITLE: Ethyl (E)-2-acetyl-3-amino-3-phenyl-2-propylenoate
AUTHOR(S): Chen, Xuanhua; Guo, Rongwei; Zhou, Zhongyuan
CORPORATE SOURCE: Department of Chemistry, Central China Normal University, Wuhan, Peop. Rep. China
SOURCE: Acta Crystallographica, Section E: Structure Reports Online (2002), E58(12), o1423-o1424
CODEN: ACSEBH; ISSN: 1600-5368
URL: http://journals.iucr.org/e/issues/2002/12/00/ww6053/index.html
PUBLISHER: International Union of Crystallography
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

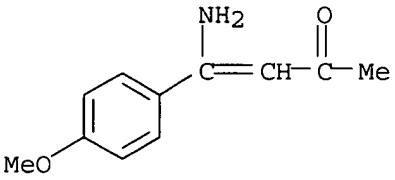
ABSTRACT:
The title compound, C13H15NO3, is an E isomer and the Ph ring does not conjugate with C=C. Both intra- and intermol. N-H...O H bonds are found, and the infinite mol. chains stretch along the b axis. Crystallog. data are given.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

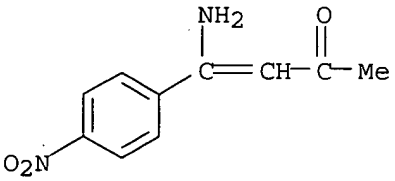
L3 ANSWER 12 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6 231301-47-6 231301-48-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective preparation of pyrazoles from β-amino enones and hydrazines)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 231301-47-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 231301-48-7 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

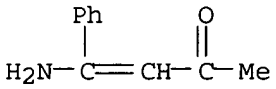


ACCESSION NUMBER: 2001:151148 CAPLUS
DOCUMENT NUMBER: 134:340457
TITLE: Scope and limitations in the regioselective synthesis of 1,3,5-trisubstituted pyrazoles from β-amino enones and hydrazine derivatives. 13C-chemical shift prediction rules for 1,3,5-trisubstituted pyrazoles
AUTHOR(S): Alberola, Angel; Bleye, Luis Calvo; Gonzalez-Ortega, Alfonso; Sadaba, M. Luisa; Sanudo, M. Carmen
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Valladolid, Valladolid, 47005, Spain
SOURCE: Heterocycles (2001), 55(2), 331-351
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:340457
ABSTRACT:

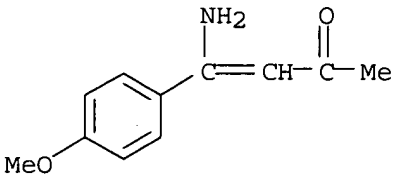
β-Amino enones react with hydrazines to give regioselectively 1,3,5-trisubstituted pyrazoles. The synthetic method only presents limitations when the β-substituent of the enone and the hydrazine substituent are bulky or possess an electron-withdrawing character. Comparison of the 13C-NMR spectra of the pyrazoles allowed for to estimate a 13C-chemical shift prediction rule
for 1,3,5-trisubstituted pyrazoles, with deviations ≤ ±1 ppm.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6 231301-47-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyrazoles via reactions of β-aminoenones with acetylhydrazine, semicarbazide and methoxycarbonylhydrazine)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 231301-47-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1999:710019 CAPLUS
DOCUMENT NUMBER: 132:93249
TITLE: Reactions of β-aminoenones with acetylhydrazine, semicarbazide and methoxycarbonylhydrazine. Synthesis of 1-acetyl-, 1-carboxamide- or methyl 1-carboxylated pyrazole derivatives
AUTHOR(S): Alberola, Angel; Calvo, Luis; Ortega, Alfonso Gonzalez; Sadaba, M. Luisa; Sanudo, M. Carmen; Granda, Santiago Garcia; Rodriguez, Elena Garcia
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Valladolid, Valladolid, 47005, Spain
SOURCE: Heterocycles (1999), 51(11), 2675-2686
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:93249
ABSTRACT:
Acetylhydrazine, semicarbazide and methoxycarbonylhydrazine react with β-aminoenones to give regioselectively the corresponding N-acetyl- or N-carboxypyrazole derivs. The reactions are highly regioselective and occur via 5-hydroxypyrazolines, which in several cases can be isolated and characterized.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN

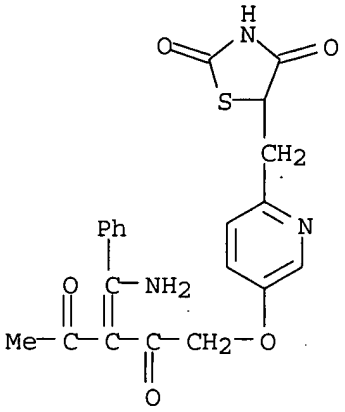
IT **243147-05-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridylmethyl(idene)thiazolidenediones as hypoglycemic agents)

RN 243147-05-9 CAPLUS

CN 2,4-Thiazolidinedione, 5-[[5-[[3-(aminophenylmethylene)-2,4-dioxopentyl]oxy]-2-pyridinyl]methyl]- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1999:606967 CAPLUS

DOCUMENT NUMBER: 131:214281

TITLE: Preparation of pyridylmethyl(idene)thiazolidenediones as hypoglycemic agents

INVENTOR(S): Ohara, Yoshio; Suzuki, Mikio; Miyachi, Nobuhide; Kato, Katsuhiro; Ohdoi, Keisuke; Kobayashi, Tetsuya; Shikada, Ken-ichi; Naito, Takeshi; Yotsumoto, Takashi

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: U.S., 74 pp., Cont.-in-part of U. S. Ser. No. 704,774, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

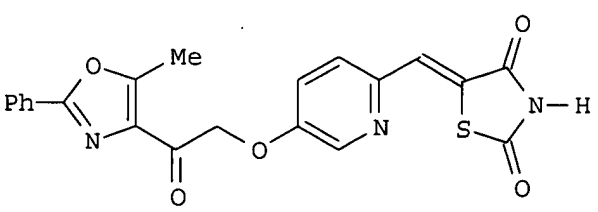
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5955481	A	19990921	US 1998-18843		19980204
ZA 9502479	A	19951215	ZA 1995-2479		19950327
PRIORITY APPLN. INFO.:			JP 1994-57192	A	19940328
			JP 1994-295177	A	19941129
			US 1995-704774	B2	19950327

OTHER SOURCE(S): MARPAT 131:214281

GRAPHIC IMAGE:

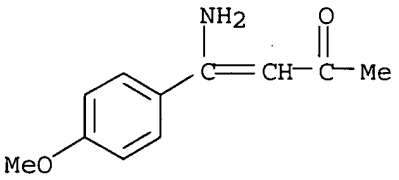


II

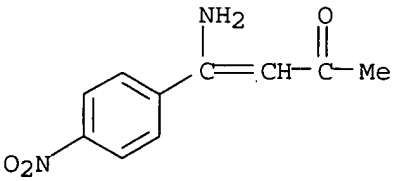
ABSTRACT:
Title compds. [I; R = R1OZ1Z2; R1 = alk(en)yl, acyl, (hetero)aryl(alkyl), etc.; R4 = H or alkyl; X = O, S, NH; Z = O or S; Z1 = (1-oxido)(un)substituted pyridine-3,6-diyl; Z2 = CR6R7 or SO2; R6,R7 = H or (cyclo)alkyl; R4R7 = bond] were prepared Thus, 5-hydroxy-2-pyridinemethanol was etherified by 4-bromoacetyl-5-methyl-2-phenyloxazole and the oxidized product condensed with thiazolidine-2,4-dione to give title compound II. Data for biol. activity of I were given.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **231301-47-6P 231301-48-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isoxazoles by ultrasound cyclocondensation of acyl enamines)
RN 231301-47-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



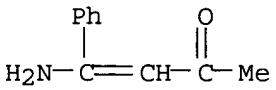
RN 231301-48-7 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



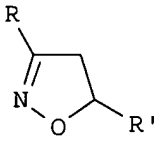
ACCESSION NUMBER: 1999:329002 CAPLUS
DOCUMENT NUMBER: 131:102226
TITLE: Reactivity of p-phenyl substituted β-enamino compounds using K-10/ultrasound. II. Synthesis of isoxazoles and 5-isoxazolones
AUTHOR(S): Valduga, Claudete J.; Santis, Denise B.; Braibante, Hugo S.; Braibante, Mara E. F.
CORPORATE SOURCE: Departamento de Quimica, Universidade Federal de Santa Maria, Santa Maria, 97105-900, Brazil
SOURCE: Journal of Heterocyclic Chemistry (1999), 36(2), 505-508
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
The condensation of 4-Ph substituted β-enamino ketones and β-enamino esters with HONH2.HCl using K-10 as the solid support under sonication was studied to evaluate the formation of isoxazole and 5-isoxazolone rings from β-enamino compds. with a substituted aromatic ring. The use of K-10/ultrasound in this reaction furnished novel results in some cases.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(iron dichloride induced isomerization and reductive cleavage of isoxazoles to carboxyazirines and enamino ketones)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1997:535658 CAPLUS
DOCUMENT NUMBER: 127:205417
TITLE: Iron dichloride induced isomerization or reductive cleavage of isoxazoles: a facile synthesis of 2-carboxyazirines
AUTHOR(S): Auricchio, Sergio; Bini, Antonella; Pastormerlo, Eros; Truscello, Ada M.
CORPORATE SOURCE: Dipartimento di Chimica, Politecnico di Milano, Milan, 20131, Italy
SOURCE: Tetrahedron (1997), 53(31), 10911-10920
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE:



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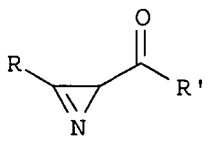
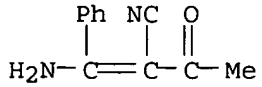


II

ABSTRACT:
5-Alkoxy-isoxazoles and N,N-disubstituted-5-isoxazolamines I (R = Ph, 4-O2NC6H4, 4-MeOC6H4, R' = OMe, NMePh, NMe2) were found to isomerize to azirine derivs. II by the use of iron dichloride as catalyst. On the contrary 5-alkyl- and 5-aryl-isoxazoles I (R = R' = Me, Ph; R = Me, R' = Ph; R = Ph, R' = Me) in the presence of the same salt, undergo reductive cleavage to enamino ketones RC(NH2):CHCOR'. A common reaction intermediate is proposed.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

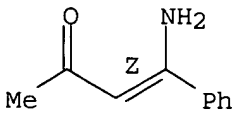
L3 ANSWER 17 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **33831-49-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of imidazo[4,5-c]pyridine derivs. with aromatic substituent as
antagonists)
RN 33831-49-1 CAPLUS
CN Butanenitrile, 2-(aminophenylmethylene)-3-oxo- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1995:741580 CAPLUS
DOCUMENT NUMBER: 123:339884
TITLE: Synthesis and evaluation of novel nonpeptide angiotensin II receptor antagonists: imidazo[4,5-c]pyridine derivatives with an aromatic substituent
AUTHOR(S): Kiyama, Ryuichi; Fuji, Masahiro; Hara, Mariko; Fujimoto, Masafumi; Kawabata, Tomoji; Nakamura, Matsuhisa; Fujishita, Toshio
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi & Co., Ltd., Osaka, 553, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(3), 450-60
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:339884
ABSTRACT:
Starting from recently reported nonpeptidic angiotensin II (AII) receptor antagonists, the authors have designed and prepared a new series of 6-arylimidazo[4,5-c]pyridine derivs. Variation of Ph groups at the 4-, 6- or 7-position of imidazo[4,5-c]pyridine showed that substitution at the 6-position resulted in receptor-binding activity almost as potent as that of DuP 753. This led to synthesis and evaluation of an extensive series of 6-aryl-imidazo[4,5-c]pyridine derivs. Some of them were 4-fold more potent in vitro than DuP 753, but only showed weak antihypertensive activity in vivo when given orally to rats.

L3 ANSWER 18 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **95514-24-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective preparation of β-enamino ketones via stereocontrolled conversion of 3-unsubstituted isoxazoles into Z-β-siloxyacrylonitriles)
RN 95514-24-2 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

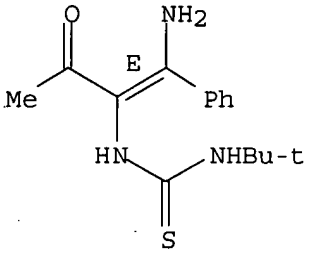


ACCESSION NUMBER: 1995:427088 CAPLUS
DOCUMENT NUMBER: 123:55070
TITLE: Stereocontrolled conversion of 3-unsubstituted isoxazole compounds into Z-β-siloxyacrylonitriles. A new method for the regioselective synthesis of β-enamino ketones
AUTHOR(S): Gonzalez, B.; Gonzalez, A. M.; Pulido, F. J.
CORPORATE SOURCE: Dep. Quim. Organ., Univ. Valladolid, Valladolid, 47011, Spain
SOURCE: Synthetic Communications (1995), 25(7), 1005-14
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Dekker

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:55070
ABSTRACT:
The stereoselective synthesis of Z-β-siloxyacrylonitriles via base-induced ring cleavage of isoxazole precursors is described. Z-β-siloxyacrylonitriles react with organolithium compds. to give high yields of β-enamino ketones.

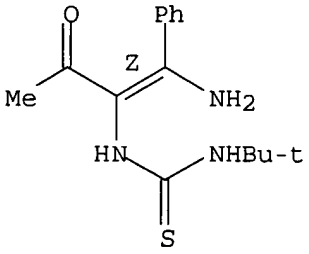
L3 ANSWER 19 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **134650-94-5P 134650-95-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 134650-94-5 CAPLUS
CN Thiourea, N-[1-(aminophenylmethylene)-2-oxopropyl]-N'-(1,1-dimethylethyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

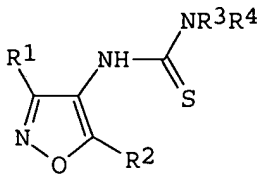


RN 134650-95-6 CAPLUS
CN Thiourea, N-[1-(aminophenylmethylene)-2-oxopropyl]-N'-(1,1-dimethylethyl)-, (Z)- (9CI) (CA INDEX NAME)

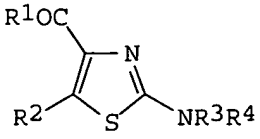
Double bond geometry as shown.



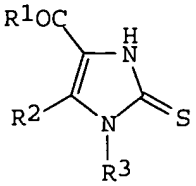
ACCESSION NUMBER: 1991:429186 CAPLUS
DOCUMENT NUMBER: 115:29186
TITLE: Transformations in the isoxazole series: synthesis of substituted 2-aminothiazoles
AUTHOR(S): Pascual, Alfons
CORPORATE SOURCE: Agro Div., Ciba-Geigy A.-G., Basel, CH-4002, Switz.
SOURCE: Helvetica Chimica Acta (1991), 74(3), 531-42
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:29186
GRAPHIC IMAGE:



I



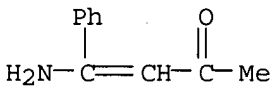
II



III

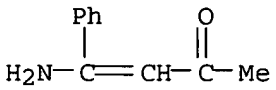
ABSTRACT:
Substituted N-(isoxazolyl)thioureas, e.g., I (R1-R4 = Me; R1-R3 = Me, R4 = Ph; R1 = R2 = Me, R3 = CMe3, PhCH2, Pr, Ph, 4-MeOC6H4, 4-MeC6H4, R4 = H; R1-R3 = CHMe2, R4 = H) undergo a transformation in the presence of hexacarbonylmolybdenum and acid to yield functionalized thiazoles, e.g., II in a one-pot reaction. In a few cases, 1,4,5-trisubstituted dihydroimidazolethiones III are also isolated as side products. Mechanistic considerations are outlined and scope and limitations of this new methodol. discussed.

L3 ANSWER 20 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(transamination of, with Et glycinate)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)

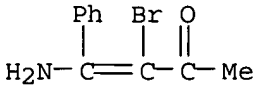


ACCESSION NUMBER: 1991:42449 CAPLUS
DOCUMENT NUMBER: 114:42449
TITLE: The reaction of β-aminoenones with α-amino derivatives. Synthesis of 2-functionalized pyrroles
AUTHOR(S): Alberola, Angel; Andres, Jose M.; Gonzalez, Alfonso; Pedrosa, Rafael; Vicente, Martina
CORPORATE SOURCE: Fac. Cienc., Univ. Valladolid, Valladolid, 47011, Spain
SOURCE: Heterocycles (1990), 31(6), 1049-58
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:42449
ABSTRACT:
β-Aminoenones react with Et glycinate, α-aminoacetonitrile and α-aminoacetamide hydrochlorides leading to 2-functionalized pyrroles. Although the transamination is a high-yield process, the transformation of the intermediate, in both basic or thermally induced conditions, affords the corresponding pyrroles in poor to moderate yields. Thus, transamination of AcCH:CMeNH2 with EtO2CCH2N+H3 in MeOH gave 89% AcCH:CMeNHCH2CO2Et which on cyclization in EtONa/EtOH gave 33% Et 3,5-dimethyl-2-pyrrolecarboxylate.

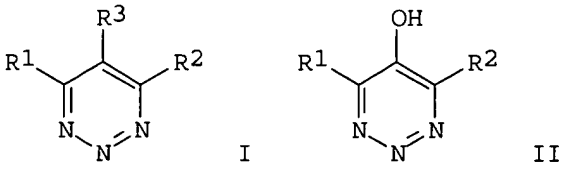
L3 ANSWER 21 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P 129200-01-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, during basic hydrolysis of bromoethylmethyltriazine)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 129200-01-7 CAPLUS
CN 3-Buten-2-one, 4-amino-3-bromo-4-phenyl- (9CI) (CA INDEX NAME)

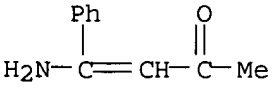


ACCESSION NUMBER: 1990:515259 CAPLUS
DOCUMENT NUMBER: 113:115259
TITLE: Reaction of 5-halo-1,2,3-triazines with superoxide; synthesis of 5-hydroxy-1,2,3-triazines
AUTHOR(S): Itoh, Takashi; Nagata, Kazuhiro; Okada, Mamiko; Ohsawa, Akio
CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Tokyo, 142, Japan
SOURCE: Tetrahedron Letters (1990), 31(17), 2429-30
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:115259
GRAPHIC IMAGE:



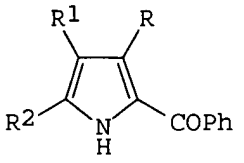
ABSTRACT:
5-Halo-1,2,3-triazines I (R1 = Me, R2 = Me, Et, Ph, R3 = Br; R1 = R2 = Et, R3 = Br; R1 = R2 = Ph, R3 = Cl) were allowed to react with electrolytically produced superoxide to give 5-hydroxy-1,2,3-triazines II. Reaction with hydroxide anion gave ring opening products, therefore this substitution was specific for superoxide.

L3 ANSWER 22 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenacylamine, acylpyrroles from)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)

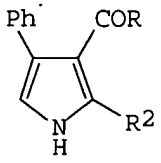


ACCESSION NUMBER: 1990:198025 CAPLUS
DOCUMENT NUMBER: 112:198025
TITLE: The reactivity of β-aminoenones towards phenacylamine hydrochloride

AUTHOR(S): Alberola, Angel; Andres, Jose M.; Gonzalez, Alfonso; Pedrosa, Rafael; Vicente, Martina
CORPORATE SOURCE: Fac. Cienc., Univ. Valladolid, Valladolid, 47011, Spain
SOURCE: Heterocycles (1989), 29(10), 1973-82
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:198025
GRAPHIC IMAGE:



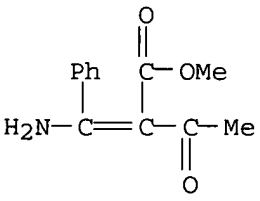
I



II

ABSTRACT:
RCOCR1:CR2NH2 (R = Me, Et, CMe3, Ph, PhCH2CH2, 4-O2NC6H4; R1 = H, Me, PhCH2, CH2CN, CO2Et, CH2CO2Et; R2= Me, Et, CMe3, Ph, PhCH2CH2) react with PhCOCH2NH2.HCl to give a mixture of 2- and 3-acylpyrroles, I and II resp. The reaction is a two-step process: formation of an isolable β-phenacylaminoenone intermediate and cyclization to 2- and 3-acylpyrroles, depending on the starting β-aminoenone substituents.

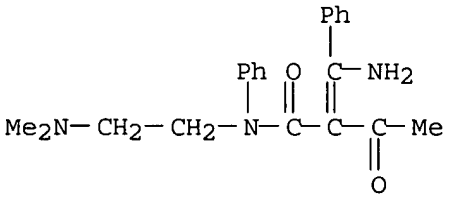
L3 ANSWER 23 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **95192-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 95192-69-1 CAPLUS
CN Butanoic acid, 2-(aminophenylmethylene)-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



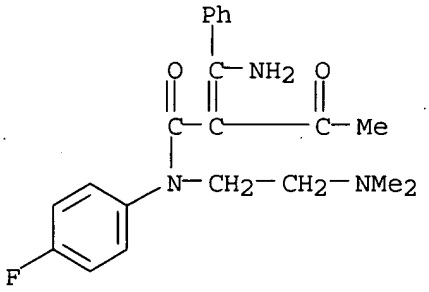
ACCESSION NUMBER: 1989:74802 CAPLUS
DOCUMENT NUMBER: 110:74802
TITLE: Tin(IV) chloride-promoted vs. metal β-carbonyl-enolate-catalyzed reactions of β-dicarbonyls with nitriles
AUTHOR(S): Veronese, Augusto C.; Gandolfi, Vittorio; Basato, Marino; Corain, Benedetto
CORPORATE SOURCE: Dip. Sci. Farm., Ferrara, 44100, Italy
SOURCE: Journal of Chemical Research, Synopses (1988), (8), 246-7
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:74802
ABSTRACT:
Acetoacetate esters underwent an addition reaction with nitriles in C6H6 or PhMe

containing SnCl4 to give MeCOC[:C(NH2)R2]CO2R1 (R1 = Me, Et; R2 = Me, Et, PhCH2, Ph, pyridyl, NH2, CO2Et, PhCO). Malonate esters CH2(CO2R3)2 (R3 = Me, Et) and R4CN (R4 = Et, NH2, CCl3, CO2Et, PhCO) gave (R3O2C)2C:C(NH2)R4.

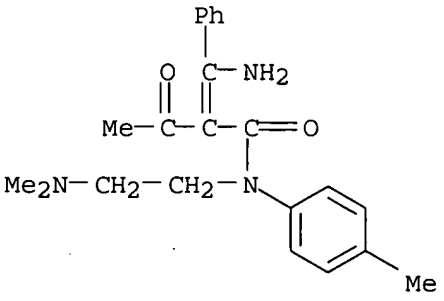
L3 ANSWER 24 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **88098-92-4P 88098-94-6P 88098-95-7P**
88098-96-8P 88098-97-9P 88098-98-0P
88098-99-1P 88099-00-7P 113702-88-8P
113702-89-9P 113702-91-3P 113702-94-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as hypoglycemic agent)
RN 88098-92-4 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



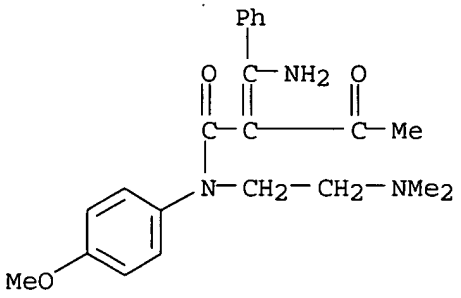
RN 88098-94-6 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-fluorophenyl)-3-oxo- (9CI) (CA INDEX NAME)



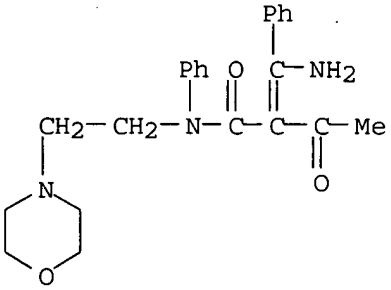
RN 88098-95-7 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-methylphenyl)-3-oxo- (9CI) (CA INDEX NAME)



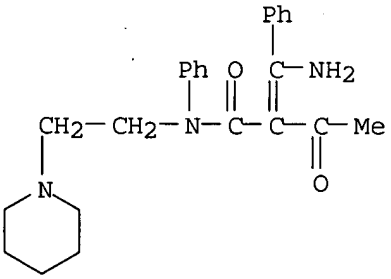
RN 88098-96-8 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-methoxyphenyl)-3-oxo- (9CI) (CA INDEX NAME)



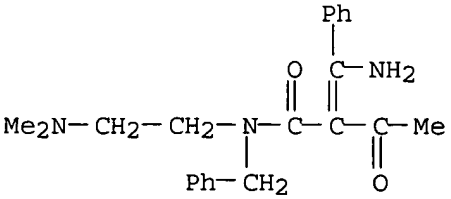
RN 88098-97-9 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(4-morpholinyl)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



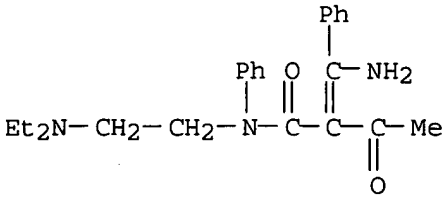
RN 88098-98-0 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-3-oxo-N-phenyl-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



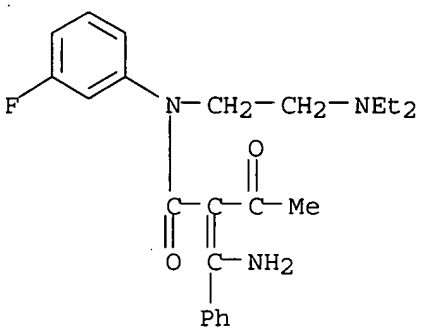
RN 88098-99-1 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-3-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 88099-00-7 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(diethylamino)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



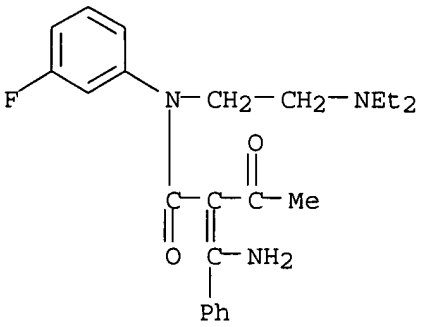
RN 113702-88-8 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(diethylamino)ethyl]-N-(3-fluorophenyl)-3-oxo- (9CI) (CA INDEX NAME)



RN 113702-89-9 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(diethylamino)ethyl]-N-(3-fluorophenyl)-3-oxo-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

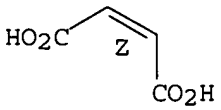
CRN 113702-88-8
CMF C23 H28 F N3 O2



CM 2

CRN 110-16-7
CMF C4 H4 O4

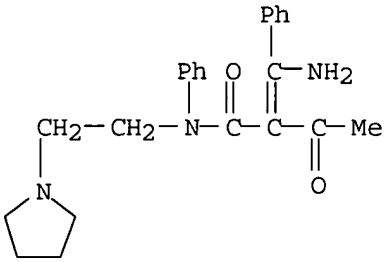
Double bond geometry as shown.



RN 113702-91-3 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-3-oxo-N-phenyl-N-[2-(1-pyrrolidinyl)ethyl]-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

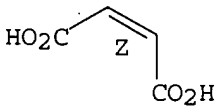
CRN 113702-90-2
CMF C23 H27 N3 O2



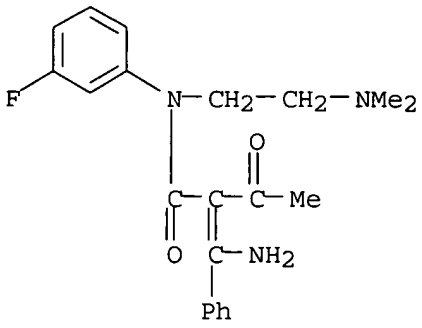
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



RN 113702-94-6 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(3-fluorophenyl)-3-oxo- (9CI) (CA INDEX NAME)

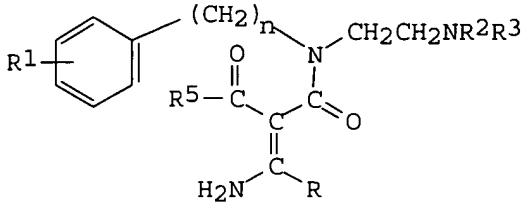


ACCESSION NUMBER: 1988:150066 CAPLUS
DOCUMENT NUMBER: 108:150066
TITLE: Preparation of N,N-disubstituted alkenamides and phenylalkenamides as antidiabetic agents

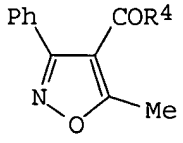
INVENTOR(S): Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz Pharmaceuticals Corp., USA
SOURCE: U.S., 8 pp. Cont.-in-part of U.S. Ser. No. 505,804, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4681898	A	19870721	US 1984-608126	19840508
PRIORITY APPLN. INFO.:			US 1981-330601 A2	19811214
			US 1983-505804 A2	19830620

OTHER SOURCE(S): CASREACT 108:150066
GRAPHIC IMAGE:



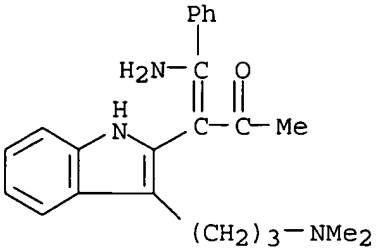
I



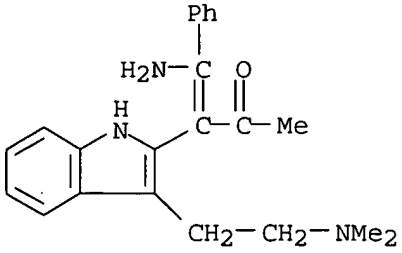
II

ABSTRACT:
The title amides [I; R = alkyl, Ph, R1C6H4; R1 = H, halo, alkyl, alkoxy; R2, R3 = alkyl; R2R3 = (CH2)4-6; R2R3N = morpholino; R5 = H, C1-6 alkyl; n = 0, 1] and their pharmaceutically acceptable salts, useful as antidiabetics and hypoglycemics, are prepared A solution of phenylisoxazole derivative II (R4 = Cl) in
THF was added to a mixture of Me2NCH2CH2NHPh and Et3N in THF under cooling and stirred at room temperature to give amide II (R4 = Me2NCH2CH2NPh), which was hydrogenated over 10% Pd-C at 50-60° and 50 psi H to give I (R = Ph, R1 = H, R2 = R3 = R5 = Me, n =0), which (350 mg) was formulated with 150 mg lactose to give a capsule showing ED25 of 74 mg/kg p.o. in treating diabetes in mammals, vs. 110 mg/kg with tolbutamide.

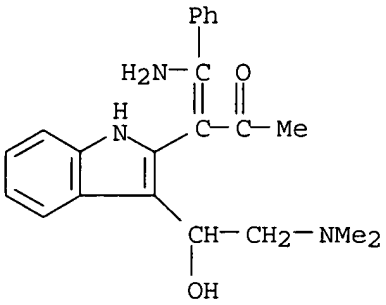
L3 ANSWER 25 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **88933-66-8 88933-68-0 100935-38-4**
100935-45-3 100935-46-4 100935-47-5
100935-48-6 100935-49-7
RL: BIOL (Biological study)
(as male contraceptive)
RN 88933-66-8 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[3-(dimethylamino)propyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



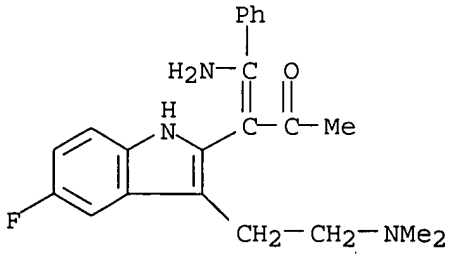
RN 88933-68-0 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)ethyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



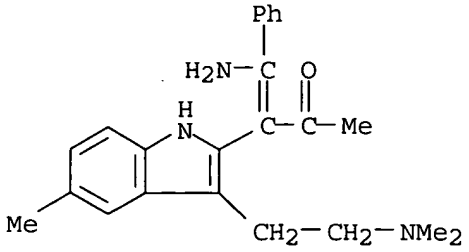
RN 100935-38-4 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)-1-hydroxyethyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



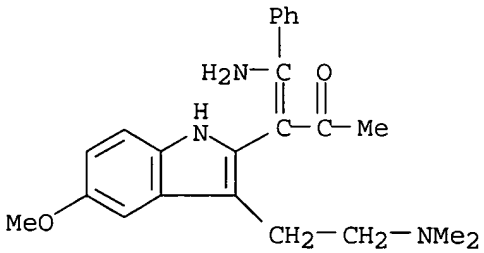
RN 100935-45-3 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)ethyl]-5-fluoro-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



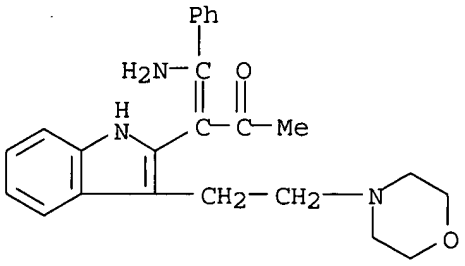
RN 100935-46-4 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)ethyl]-5-methyl-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



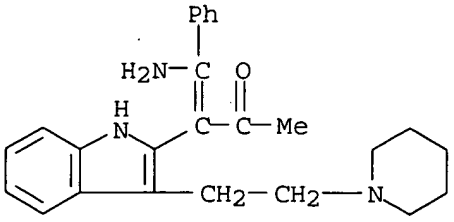
RN 100935-47-5 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)ethyl]-5-methoxy-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 100935-48-6 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(4-morpholinyl)ethyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 100935-49-7 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-3-[3-[2-(1-piperidinyl)ethyl]-1H-indol-2-yl]- (9CI) (CA INDEX NAME)

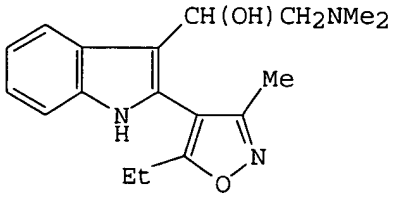


ACCESSION NUMBER: 1986:116097 CAPLUS
DOCUMENT NUMBER: 104:116097
TITLE: Indolamine derivatives as anti-fertility agents
INVENTOR(S): Manning, Robert E.; Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz, Inc., USA

SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4544663	A	19851001	US 1984-607667	19840507

PRIORITY APPLN. INFO.: US 1984-607667 19840507
GRAPHIC IMAGE:

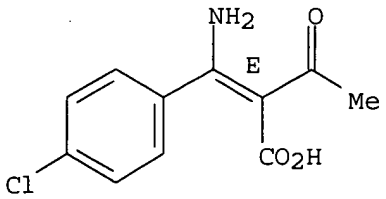


I

ABSTRACT:
Ninety indolamines were tested for aspermatogenic activity in adult beagle dogs. A representative compound I caused a significant decrease in spermatogenesis after 14 days of oral administration at 12 mg/kg/day in the dogs. The effect lasted for .apprx.85 days. Histopathol. examns. of testes were normal. Tablets and capsules composition are also described.

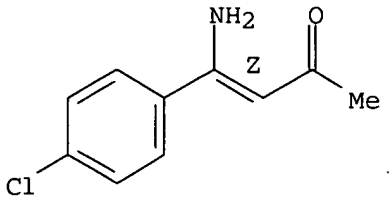
L3 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **95514-22-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)
RN 95514-22-0 CAPLUS
CN Butanoic acid, 2-[amino(4-chlorophenyl)methylene]-3-oxo-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



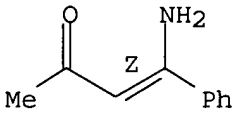
IT **95514-23-1P 95514-24-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring closure of)
RN 95514-23-1 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(4-chlorophenyl)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 95514-24-2 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



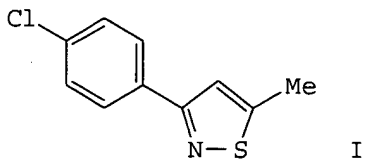
ACCESSION NUMBER: 1985:166113 CAPLUS
DOCUMENT NUMBER: 102:166113

TITLE: Ring transformation equilibrium (bond switch) in 5-(2-aminovinyl)isothiazole system via hypervalent sulfurane. Synthesis, structure determination, and kinetic study

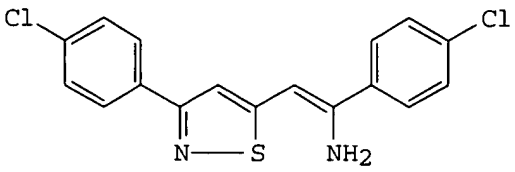
AUTHOR(S): Akiba, Kinya; Kashiwagi, Kohichi; Ohyama, Yoshihiko; Yamamoto, Yohsuke; Ohkata, Katsuo
CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan

SOURCE: Journal of the American Chemical Society (1985), 107(9), 2721-30
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:166113

GRAPHIC IMAGE:



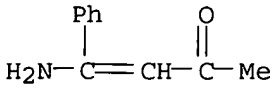
I



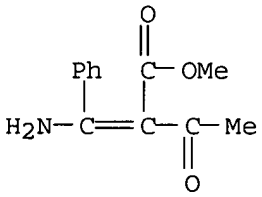
II

ABSTRACT:
Reaction of 3-aryl-5-methylisothiazoles (e.g. I) with aromatic nitriles afforded (aminovinyl)isothiazoles (e.g. II) in the presence of LDA. The ring transformation of (aminovinyl)isothiazoles was studied. Rates of reversible ring transformation for the (aminovinyl)isothiazoles were determined; solvent and substituent effects were discussed.

L3 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P 95192-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)

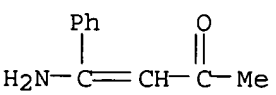


RN 95192-69-1 CAPLUS
CN Butanoic acid, 2-(aminophenylmethylene)-3-oxo-, methyl ester (9CI) (CA INDEX NAME)



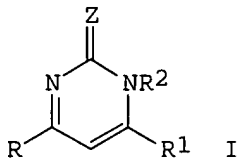
ACCESSION NUMBER: 1985:149156 CAPLUS
DOCUMENT NUMBER: 102:149156
TITLE: Reduction of cyclic compounds having nitrogen-oxygen linkage by dihydrolipoamide-iron(II)
AUTHOR(S): Kijima, Masashi; Nambu, Yoko; Endo, Takeshi
CORPORATE SOURCE: Res. Lab. Resour. Util., Tokyo Inst. Technol., Yokohama, 227, Japan
SOURCE: Journal of Organic Chemistry (1985), 50(7), 1140-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:149156
ABSTRACT:
Dihydrolipoamide (DHLAm) was an effective reagent in the presence of a catalytic amt of Fe2+ for the reduction of cyclic N-O compds. such as isoxazolidines and isoxazoles. Isoxazolidines and isoxazoles were reduced to 3-aminopropanols and β-aminoenones in good yields, resp. The reduction might proceeds through the complex formation between DHLAm-Fe(II) and N-O compds.

L3 ANSWER 28 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn.-cyclocondensation of, with aryl isocyanates and isothiocyanates)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1984:423428 CAPLUS
Correction of: 1983:198136

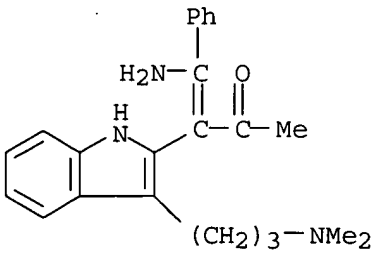
DOCUMENT NUMBER: 101:23428
Correction of: 98:198136
TITLE: The selective synthesis of unsymmetrical 1-substituted 2(1H)-pyrimidinones and -thiones
AUTHOR(S): Kashima, Choji; Katoh, Akira; Yokota, Yuko; Omote, Yoshimori
CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Sakura, 305, Japan
SOURCE: Synthesis (1983), (2), 151-3
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE:



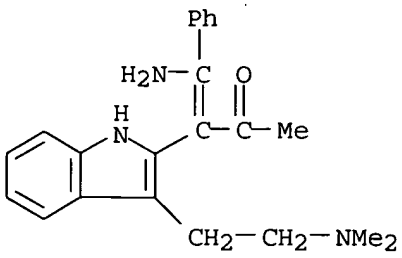
I

ABSTRACT:
The reaction of RC(NH2):CHCOR1 (R = Me, Et, Ph; R1 = C1-3 alkyl, Ph) with R2N:C:Z (R2 = Ph, 4-ClC6H4, Et; Z = O, S) and NaH yielded pyrimidines I. Thus, MeC(NH2):CHCOEt was treated with PhNCO and NaH in DMF at room temperature to give I (R = Me, R1 = Et, R2 = Ph, Z = O). Ketone MeC(NH2):CHCOMe and PhNCS gave MeC(NH2):C(CSNHPh)COMe and only a small amount of I (R = R1 = Me, R2 = Ph, Z = S).

L3 ANSWER 29 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **88933-66-8P 88933-68-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antidiabetic)
RN 88933-66-8 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[3-(dimethylamino)propyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



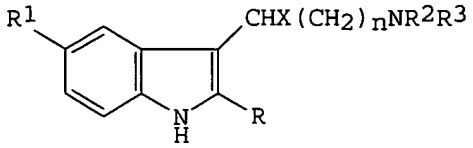
RN 88933-68-0 CAPLUS
CN 3-Buten-2-one, 4-amino-3-[3-[2-(dimethylamino)ethyl]-1H-indol-2-yl]-4-phenyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1984:156590 CAPLUS
DOCUMENT NUMBER: 100:156590
TITLE: 2-Substituted-3-indolamines and their use
INVENTOR(S): Brand, Leonard Jay; Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3312107	A1	19831020	DE 1983-3312107	19830402
CH 656124	A	19860613	CH 1983-1761	19830330
US 4536499	A	19850820	US 1983-481373	19830401
FI 8301165	A	19831014	FI 1983-1165	19830406
BE 896421	A1	19831011	BE 1983-10756	19830411
DK 8301592	A	19831014	DK 1983-1592	19830411
FR 2524881	A1	19831014	FR 1983-5992	19830411
FR 2524881	B1	19850920		
GB 2119372	A1	19831116	GB 1983-9729	19830411
GB 2119372	B2	19850918		
SE 8302026	A	19831014	SE 1983-2026	19830412
AU 8313440	A1	19831020	AU 1983-13440	19830412
JP 58188882	A2	19831104	JP 1983-63100	19830412
HU 32560	O	19840828	HU 1983-1273	19830412
ES 521398	A1	19841101	ES 1983-521398	19830412
NL 8301289	A	19831101	NL 1983-1289	19830413
ZA 8302600	A	19841128	ZA 1983-2600	19830413
US 4582848	A	19860415	US 1983-504941	19830616
PRIORITY APPLN. INFO.:			US 1982-367938 A	19820413
			US 1982-387224 A	19820610

OTHER SOURCE(S): CASREACT 100:156590
GRAPHIC IMAGE:



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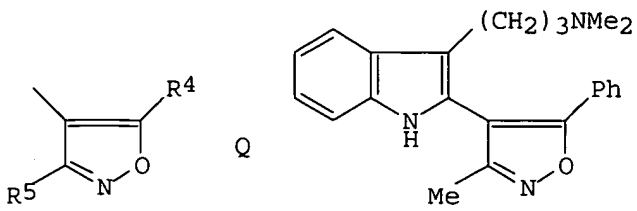
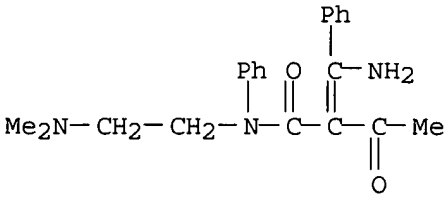


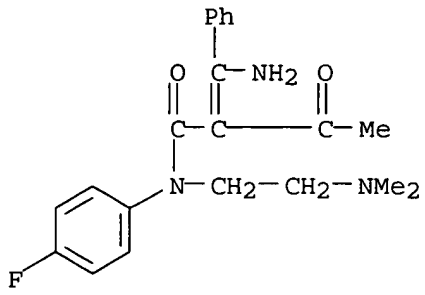
II

ABSTRACT:
Indolamines I [R1 = H, F, Cl, C1-4 alkyl or alkoxy; R2, R3 = C1-4 alkyl; NR2R3 = pyrrolidino, piperidinyl, hexamethylenimino, morpholino; R = Q, X = H, n = 2-4; R = C6H4Ph, naphthyl, C6H4CH2Ph, indanyl, fluorenyl, C(COR4):C(NH2)R5, X = H or OH n = 1-4; R4 = H, C1-4 alkyl; R5 = H, C1-4 alkyl, Ph (un)substituted with halogen, C1-4 alkyl or alkoxy] and their acid addition salts, useful as antidiabetics (no data), were prepared Isoxazolylindolepropanamine II was prepared in 6 steps from 2-(5-methyl-3-phenyl-4-isoxazolyl)indole, HNMe2, and 37% aqueous HCHO.

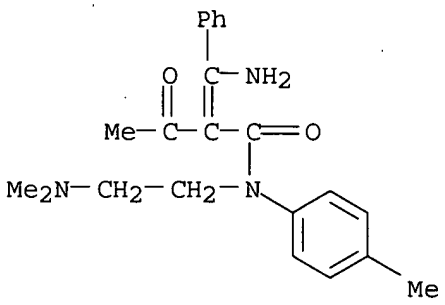
L3 ANSWER 30 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **88098-92-4P 88098-94-6P 88098-95-7P**
88098-96-8P 88098-97-9P 88098-98-0P
88098-99-1P 88099-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 88098-92-4 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



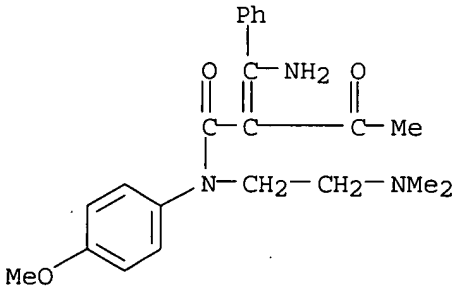
RN 88098-94-6 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-fluorophenyl)-3-oxo- (9CI) (CA INDEX NAME)



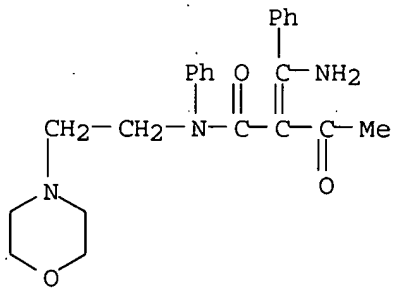
RN 88098-95-7 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-methylphenyl)-3-oxo- (9CI) (CA INDEX NAME)



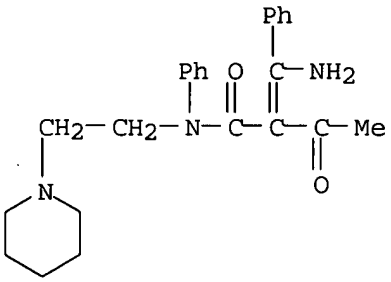
RN 88098-96-8 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-N-(4-methoxyphenyl)-3-oxo- (9CI) (CA INDEX NAME)



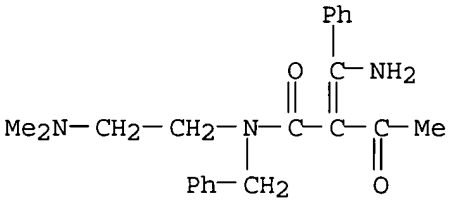
RN 88098-97-9 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(4-morpholinyl)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



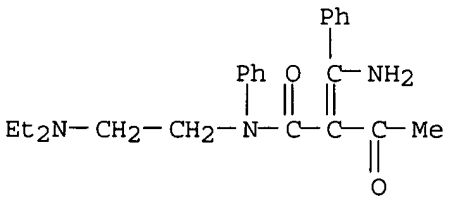
RN 88098-98-0 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-3-oxo-N-phenyl-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 88098-99-1 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(dimethylamino)ethyl]-3-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 88099-00-7 CAPLUS
CN Butanamide, 2-(aminophenylmethylene)-N-[2-(diethylamino)ethyl]-3-oxo-N-phenyl- (9CI) (CA INDEX NAME)



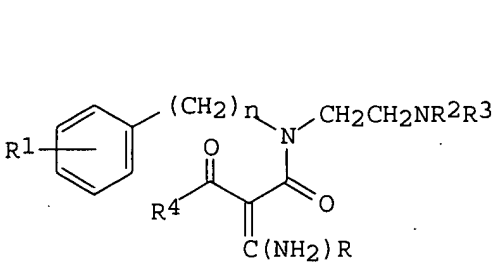
ACCESSION NUMBER: 1984:6099 CAPLUS
DOCUMENT NUMBER: 100:6099
TITLE: N,N-Disubstituted alkenamides and phenylalkenamides and their use as pharmaceuticals
INVENTOR(S): Nadelson, Jeffrey
PATENT ASSIGNEE(S): Sandoz A.-G., Switz.; Sandoz-Patent-G.m.b.H.; Sandoz-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 84292	A1	19830727	EP 1982-810533	19821209
EP 84292	B1	19850213		

R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE

AT 11770	E	19850215	AT 1982-810533		19821209
DK 8205534	A	19830615	DK 1982-5534		19821213
JP 58110549	A2	19830701	JP 1982-219144		19821213
HU 27472	O	19831028	HU 1982-4019		19821213
HU 189626	B	19860728			
CA 1191511	A1	19850806	CA 1982-417542		19821213
IL 67464	A1	19860831	IL 1982-67464		19821213
FI 8204298	A	19830615	FI 1982-4298		19821214
AU 8291476	A1	19830623	AU 1982-91476		19821214
AU 561008	B2	19870430			
ES 518186	A1	19840601	ES 1982-518186		19821214
ZA 8209190	A	19840725	ZA 1982-9190		19821214
PRIORITY APPLN. INFO.:			US 1981-330601	A	19811214
			EP 1982-810533	A	19821209

GRAPHIC IMAGE:



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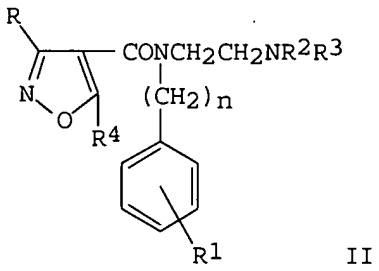
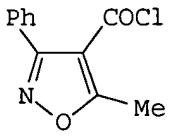


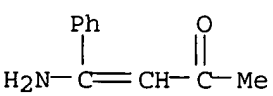
II



III

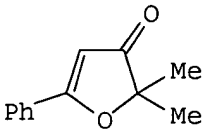
ABSTRACT:
Title amides I [R = C1-4 alkyl, substituted Ph; R1 = halo, C1-4 alkyl, C1-4 alkoxy; R2, R3 = C1-4 alkyl; R2R3 = (CH2)m (m = 4, 5, 6), CH2CH2OCH2CH2; R4 = H, C1-6 alkyl; n = 0, 1], useful as antidiabetics (no data), were prepared by the reductive cleavage of isoxazoles II. Thus,PhNHCH2CH2NMe2 was acylated with acid chloride III in THF containing Et3N to give II (R = Ph, R1 = H, R2-R4 = Me, n = 0), which was cleaved by hydrogenolysis over Pd/C to give I (R = Ph, R1 = H, R2-R3 = Me, n = 0).

L3 ANSWER 31 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1983:505069 CAPLUS
DOCUMENT NUMBER: 99:105069
TITLE: Reduction of Δ2-isoxazolines. 2. A facile

	synthesis of 3(2H)-furanones
AUTHOR(S):	Curran, Dennis P.; Singleton, David H.
CORPORATE SOURCE:	Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE:	Tetrahedron Letters (1983), 24(20), 2079-82 CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 99:105069
GRAPHIC IMAGE:	



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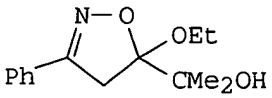
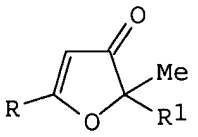


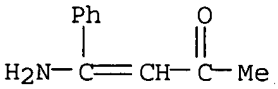
II



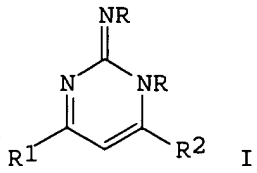
III

ABSTRACT:
The 3(2H)-furanone ring system, a structural unit of natural products such as bullatenone (I), geiparvarin, jatrophone, and lychnophorolide, was prepared by cycloaddn. of a nitrile oxide and enol ether and hydrogenolysis-hydrolysis of the resulting isoxazoline. Thus, cyclization of HOCMe2C(OEt):CH2 and PhC.tplbond.N+O- (generated in situ from PhCH2NO2 and PhNCO-Et3N), gave the isoxazoline II. Hydrogenolysis of II gave HOCMe2COCH:C(NH2)Ph which was not isolated and hydrolyzed to give I. Furanones III (R = Me, Et; R1 = Me, HOCH2CH2, HOCH2CH2CH2, H) were prepared analogously.

L3 ANSWER 32 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with carbodiimides, pyrimidines from)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER:	1983:470667 CAPLUS
DOCUMENT NUMBER:	99:70667
TITLE:	A convenient synthesis of 4,6-disubstituted 1-aryl-2-arylimino-1,2-dihydropyrimidines
AUTHOR(S):	Katoh, Akira; Sagane, Masako; Omote, Yoshimori; Kashima, Choji
CORPORATE SOURCE:	Dep. Chem., Univ. Tsukuba, Ibaraki, 305, Japan
SOURCE:	Synthesis (1983), (5), 409-10 CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 99:70667
GRAPHIC IMAGE:	



I

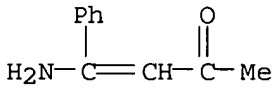
ABSTRACT:
Cyclization of carbodiimides RN:C:NR (R = Ph, p-tolyl) with α,β-unsatd. β-amino ketones R1C(NH2):CHCOR2 (R1 = Me, Ph; R2 = Me, Pr, Ph, p-ClC6H4) gave 36-92% title compds. I.

L3 ANSWER 33 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN

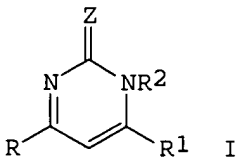
IT **14088-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn.-cyclocondensation of, with aryl isocyanates and isothiocyanates)

RN 14088-41-6 CAPLUS

CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1983:198136 CAPLUS
DOCUMENT NUMBER: 98:198136
TITLE: The selective synthesis of unsymmetrical 1-substituted 2(1H)-pyrimidinones and -thiones
AUTHOR(S): Kashima, Choji; Katoh, Akira; Yokota, Yuko; Omote, Yoshimori
CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Sakura, 305, Japan
SOURCE: Synthesis (1983), (2), 151-3
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:198136
GRAPHIC IMAGE:

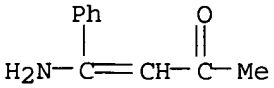


I

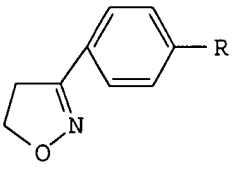
ABSTRACT:
The reaction of RC(NH2):CHCOR1 (R = Me, Et, Ph; R1 = C1-3 alkyl, Ph) with R2N:C:Z (R2 = Ph, 4-ClC6H4, Et; Z = O, S) and NaH yielded pyrimidines I. Thus, MeC(NH2):CHCOEt was treated with PhNCO and NaH in DMF at room temperature to give I (R = Me, R1 = Et, R2 = Ph, Z = O). Ketone MeC(NH2):CHCOMe and PhNCS gave MeC(NH2):C(CSNHPh)COMe and only a small amount of I (R = R1 = Me, R2 = Ph, Z = S).

L3 ANSWER 34 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN

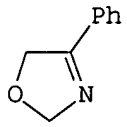
IT **14088-41-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



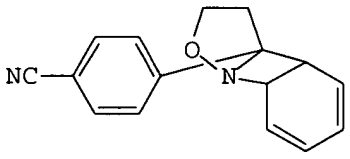
ACCESSION NUMBER: 1982:84853 CAPLUS
DOCUMENT NUMBER: 96:84853
TITLE: Organic photochemistry. Part 50. Photochemistry of 3-aryl-2-isoxazoline
AUTHOR(S): Kumagai, T.; Shimizu, K.; Kawamura, Y.; Mukai, T.
CORPORATE SOURCE: Dep. Chem., Tohoku Univ., Sendai, 980, Japan
SOURCE: Tetrahedron (1981), 37(19), 3365-76
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:84853
GRAPHIC IMAGE:



I



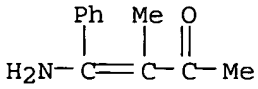
III



IV

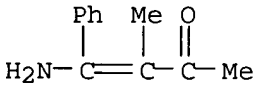
ABSTRACT:
Irradiation of the isoxazoline I (R = H) (II) in C6H6 for 12 h gave oxazoline III, PhC(:NH)CH2CHO, and PhCN in 5, 62, and 24% yield, resp. Analogous products were obtained on irradiation of I (R = Me, MeO, CN, Cl) and of 3-(2-thienyl)-2-isoxazoline. The mechanisms of these reactions involve N-O bond cleavage of the π-π^* singlet excited state of II. The absorption and emission spectra of II and of the related compds. 2-phenyl-1-pyrrolidine, 4-phenyl-3-oxazoline, and 2-phenyl-2-oxazoline were recorded and discussed. I (R = CN) formed the 1:1 photoadduct IV with C6H6.

L3 ANSWER 35 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **78052-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with disulfur dichloride)
RN 78052-25-2 CAPLUS
CN 3-Buten-2-one, 4-amino-3-methyl-4-phenyl- (9CI) (CA INDEX NAME)

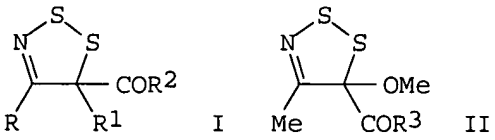


ACCESSION NUMBER: 1982:68907 CAPLUS
DOCUMENT NUMBER: 96:68907
TITLE: Reactions of ketone hydrazones and β-keto enamines with disulfur dichloride. New synthesis of thioketones and 5H-1,2,3-dithiazoles
AUTHOR(S): Okazaki, Renji; Inoue, Kaoru; Inamoto, Naoki
CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1981), 54(11), 3541-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Treating ketone hydrazones with S2Cl2 in the presence of NEt3 gave thioketones in good yields, probably via sulfinylamines R2C:NN:S:S and S-thioxothioketones R2C:S:S. The formation of di-tert-Bu and di-1-adamantyl thioketones even at low temps. suggests that steric congestion alone does not stabilize the S-thioxothioketones. Treating β-ketoenamines with S2Cl2 gives 5H-1,2,3-dithiazoles via intramol. cyclization of intermediary N-thiosulfinylamines.

L3 ANSWER 36 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **78052-25-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with disulfur dichloride, dithiazole derivative from)
RN 78052-25-2 CAPLUS
CN 3-Buten-2-one, 4-amino-3-methyl-4-phenyl- (9CI) (CA INDEX NAME)



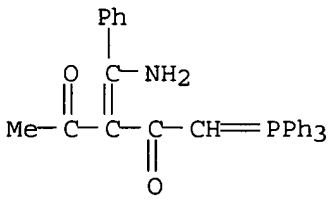
ACCESSION NUMBER: 1981:424930 CAPLUS
DOCUMENT NUMBER: 95:24930
TITLE: Synthesis of 5H-1,2,3-dithiazole, a novel heterocycle
AUTHOR(S): Okazaki, Renji; Inoue, Kaoru; Inamoto, Naoki
CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Heterocycles (1981), 15(2), 803-6
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE:



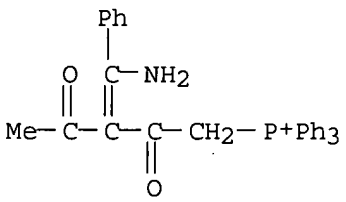
ABSTRACT:
The dithiazoles I [R = R1 = R2 = Me, RR1 = (CH2)4, R2 = EtO; R = Ph, R1 = R2 = Me] were prepared by reaction of S2Cl2 with H2NCR:CR1COR2. H2NCMe:CHCOR3 (R3 =

Me, EtO) reacted with S2Cl2 in MeOH containing Et3N to give the dithiazoles II.

L3 ANSWER 37 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **58752-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)
RN 58752-17-3 CAPLUS
CN 2,4-Pentanedione, 3-(aminophenylmethylene)-1-(triphenylphosphoranylidene)-(9CI) (CA INDEX NAME)



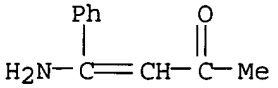
IT **58752-12-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrobromination of)
RN 58752-12-8 CAPLUS
CN Phosphonium, [3-(aminophenylmethylene)-2,4-dioxopentyl]triphenyl-, bromide (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1976:105690 CAPLUS
DOCUMENT NUMBER: 84:105690
TITLE: New α,γ-dicarbonyl-γ'-enamino-substituted methylenephosphoranes. α,γ,γ'-Tricarbonyl olefins
AUTHOR(S): Bravo, Pierfrancesco; Ticozzi, Calimero
CORPORATE SOURCE: Ist. Chim., Politech. Milano, Milan, Italy
SOURCE: Chemistry & Industry (London, United Kingdom) (1975), (23), 1018-19
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Bromination of isoxazoles (I, R = H, R1 = Me, Et, Ph; R = Me, R1 = Me, Ph) gave the 4-bromoacetyl derivative which reacted with Ph3P in C6H6 to give 80-95% of the corresponding phosphonium salt which underwent ring cleavage by H/Raney Ni, giving H2NCR1:C(COR)COCH2P+Ph3.Br- which was dehydrobrominated by BuLi or aqueous NaOH-EtOH to the ylide H2NCR1:C(COR)COCH:PPh3 (II). Reaction of II with p-R2C6H4CHO (R2 = H, OMe, NO2) gave 80-90% H2NCR1:(CHO)COCH:CHC6H4R2-p which

were hydrolyzed in aqueous HCl to olefins R1COCH(CHO)COCH:CHC6H4R2-p.

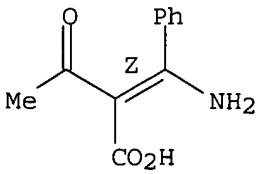
L3 ANSWER 38 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1975:409870 CAPLUS
DOCUMENT NUMBER: 83:9870
TITLE: Isoxazolylmethylenedimethylsulfonium ylids
AUTHOR(S): Bravo, Pierfrancesco; Gaviraghi, Giovanni
CORPORATE SOURCE: Ist. Chim., Politec. Milan, Milan, Italy
SOURCE: Gazzetta Chimica Italiana (1974), 104(11-12), 1307-9
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 83:9870
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The reaction of ylide I (R = H) (II) with R1R2CO gave epoxyalkylisoxazoles III (X = O, R1 = H, R2 = Ph, p-tolyl, p-anisyl, p-ClC6H4; R1 = R2 = Ph). The acylation of II with BzCl gave I (R = Bz). The Michael addition of BzCH:CHPh to II gave cyclopropylisoxazole III (X = PhCH, R1 = H, R2 = Bz).

L3 ANSWER 39 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **40030-32-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40030-32-8 CAPLUS
CN Butanoic acid, 2-(aminophenylmethylene)-3-oxo-, (Z)- (9CI) (CA INDEX NAME)

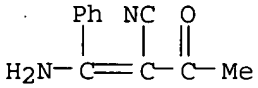
Double bond geometry as shown.



ACCESSION NUMBER: 1973:97531 CAPLUS
DOCUMENT NUMBER: 78:97531
TITLE: Hydrogenation of 2-isoxazolin-5-ones
AUTHOR(S): Mueller, Werner; Kraatz, Udo; Korte, Friedhelm
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1973), 106(1), 332-8
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Hydrogenation of the title compds. (I, R = Me or Ph; R1 = H or Et; II, R2, R3 =

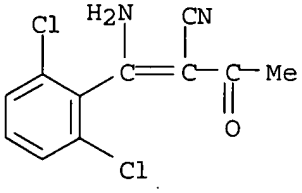
H or Me; and III, R2 = Me or Ph) over Pd-C gave Ph(H2N)C:C(COR)CO2H. Hydrogenation of II gave the diazepines IV. Similarly, III (R2 = Ph) and III (R2 = Me) gave the pyrazole derivs. V and VI, resp.

L3 ANSWER 40 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **33831-49-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33831-49-1 CAPLUS
CN Butanenitrile, 2-(aminophenylmethylene)-3-oxo- (9CI) (CA INDEX NAME)

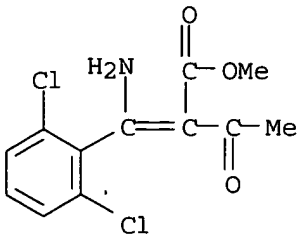


ACCESSION NUMBER: 1971:529619 CAPLUS
DOCUMENT NUMBER: 75:129619
TITLE: Ketene and its derivatives. XLIII. Reaction of primary enamines with ketene and diketene
AUTHOR(S): Kato, Tetsuzo; Yamanaka, Hiroshi; Hozumi, Toyoharu
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE: Yakugaku Zasshi (1971), 91(7), 740-9
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Reaction of primary enamines, such as 3-amino-crotononitrile (I), β-aminocinnamonitrile (II), 4-amino-3-penten-2-one (III), and ethylβ-aminocinnamate (IV), with ketene resulted in acylation of the enamine-C to give C-acetates or C,N-diacetates. Acetylation of I-IV with Ac2O gave the N-acetates, whose reaction with ketene did not afford C,N-diacetates. I-IV reacted with diketene and the enamine-C and N were both acylated, giving 2,3-disubstituted 6-methyl-4-pyridinols (e.g. V), N-acetoacetate, and 2,6-dimethyl-4-oxopyran-3-carboxamide derivs. (e.g. VI). Similar results were obtained with other enamines, e.g. ethyl 3-aminocrotonate, 3-amino-2-cyclohexen-1-one, and 3-amino-5,5-dimethyl-2-cyclohexen-1-one.

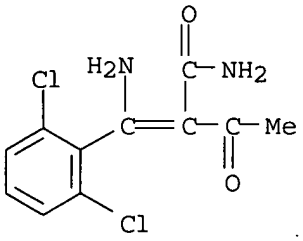
L3 ANSWER 41 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **21486-59-9P 21486-61-3P 21486-62-4P**
23706-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21486-59-9 CAPLUS
CN Cinnamonitrile, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



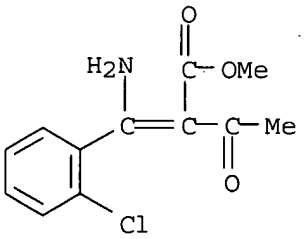
RN 21486-61-3 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-2,6-dichloro-, methyl ester (8CI) (CA INDEX NAME)



RN 21486-62-4 CAPLUS
CN Cinnamamide, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



RN 23706-89-0 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-o-chloro-, methyl ester (8CI) (CA INDEX NAME)



ACCESSION NUMBER: 1969:501850 CAPLUS
DOCUMENT NUMBER: 71:101850
TITLE: Isothiazoles
INVENTOR(S): Cheney, Lee C.; Crast, Leonard B., Jr.
PATENT ASSIGNEE(S): Bristol-Myers Co.
SOURCE: Fr., 12 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

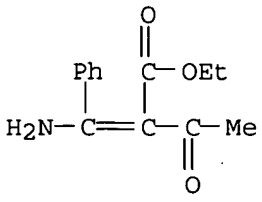
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1535810		19680809		
DE 1670249			DE	
GB 1174841			GB	
PRIORITY APPLN. INFO.:			US	19660725

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The title compds. (I), useful as intermediates for synthetic penicillins, are prepared Thus, a mixture of 200 g. Me 3-(2,6-dichlorophenyl)-5-methylisoxazole-4-

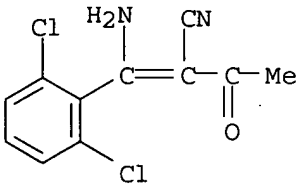
carboxylate, 50 g. Raney Ni, and 1.1 l. MeOH was hydrogenated 12 hrs. with 3.5 atmospheric H to yield 59.6% 1-amino-2-carbomethoxy-1-(2,6-dichlorophenyl)-1-buten-3-one (II), m. 155-6° (PhMe). To 110 g. II in 500 ml. C6H6 was added 160 g. PCl5 with stirring, the mixture stirred 3 hrs. at room temperature, worked up, the product dissolved in 100 ml. C6H6, the mixture added at 5-10° to 100 g. NaSH.xH2O in 1 l. dry MeOH, H2S is bubbled through 1 hr., the mixture is stirred 16 hrs. at room temperature, and worked up to yield an oil which is dissolved in 250 ml. CH2Cl2. To this solution is added with stirring 62.4 g. K2CO3 and a solution of 96.14 g. iodine in 2.5 l. CH2Cl2 is added in 45 min. at room temperature; stirring is continued 30 min. and the mixture is worked up to yield a residue which is saponified by refluxing 1 hr. with a solution of 32 g. NaOH in 400 ml. 50% aqueous MeOH to yield I (R = 2,6-Cl2C6H3, R1 = Me) (III), m. 215-17°. Also prepared are 1-amino-2-carbethoxy-1-phenyl-1-buten-3-one, m. 76-7° (PhMe), and I (R = Ph, R1 = Me) (IV), m. 154-4.5°. A mixture of 3.2 g. IV and 5 ml. SOCl2 is heated 1 hr. at 70-80° to yield 95% of the acid chloride, b0·6 122-5°, which is dissolved in 5 ml. CH2Cl2 and added in 2 min. with stirring at 5-10° to a solution of 3 g. 6-aminopenicillanic acid and 3 g. Et3N in 50 ml. CH2Cl2; the mixture is stirred 1 hr. at 15° to yield 39% Na-6-(5-methyl-3-phenylisothi azole-4-carboxamido)penicillanate H2O (V), m. 184-90° (decomposition). A solution of 175 g. 3-(2-chlorophenyl)-5-methyl-4-isoxazolecarboxylic acid chloride in 1 l. MeOH is refluxed 5 hrs. to yield 78.8% Me 3-(2-chlo rophenyl)-5-methyl-4-isoxazolecarboxylate, m. 58-9° (MeOH), which is converted via 57.5% 1-amino-2-carbomethoxy-1-(2-chlorophenyl)-1-bu ten-3-one, m. 89-91°, into I (R = 2-ClC6H4, R1 = Me), m. 185-7°. A solution of 50 g. 3-(2,6-dichlorophenyl)-5-methyl-4-isoxazolecarboxylic acid chloride in 300 ml. tetrahydrofuran is added to 300 ml. concentrated aqueous NH4OH and the mixture is kept 18 hrs. at 25° to yield 61% 4-carba moyl-3-(2,6-dichlorophenyl)-5-methylisoxazole (VI), m. 166° (EtOH-H2O). A mixture of 26 g. VI, 36 ml. Et3N, and 200 ml. POCl3 is refluxed 2 hrs. to yield 80% 4-cyano-3-(2,6-dichlorophenyl)-5-methylisoxazole (VII), m. 99-100° (iso-PrOH-H2O). VII is converted as described for III via 1-amino-2-cyano-1-(2,6-dichlorophenyl)-1-buten-3-one, m. 231-2°, into 4-cyano-3-(2,6-dichlorophenyl)-5-methylisothiazole (VIII), m. 125-6°. A mixture of 729.5 mg. VIII, 3.3 ml. ethylene glycol, 0.66 ml. H2O and 0.33 g. KOH is refluxed 49 hrs. to yield 86% III. VI is converted as described for II into 1-amino-2-carbamoyl-1-(2,6- dichlorophenyl)-1-buten-3-one, m. 226-8° (iso-PrOH-H2O), which is converted into III. To a mixture of 37.8 g. 2,6-Cl2C6H3CH:NOH and 200 ml. H2O is added gradually with stirring at 5-10° 425 ml. aqueous solution containing 0.2 mole NaOCl, the mixture is stirred 0.5 hr. and worked up to yield a residue which is dissolved in 200 ml. anhydrous EtOH. To this solution is added with stirring at 5° 30 g. EtCOCH2CO2Et and a solution of 1.76 g. NaOH in 40 ml. EtOH to yield 53.5% Et 3-(2,6-dichlorophenyl)-5-ethyl-4-isoxazolecarboxylate, m. 62-3°, which is converted via 83% 1-amino-2-carbethoxy-1-(2,6-dichlorophenyl)-1-pen ten-3-one, m. 109.5-10.5°, into I (R = 2,6-Cl2C6H3, R1 = Et), m. 206-8°. Also prepared were: 3-(2-chloro-6-fluorophenyl)-5-methyl-4-isoxazolecarboxylic acid, m. 205-6° (EtOH-H2O) (Me ester m. 55-6°); I [R = 2,6-Cl(F)C6H3, R1 = Me], m. 199-201°; Na 6-[3-2-chloro-6-fluorophenyl)-5-methyl-4-isothiazolecarboxa-mido]-penicillanate-H2O, m. 175-6° (decomposition); and the following I (R1 = Me) (R given): Me (m. 180-200°); 2,6-dichloro-4-methylphenyl; 2,4,6-Cl3C6H2; 2-chloro-6-fluoro-4-methoxyphenyl; 4-F3CC6H4; 2,6-(F3C)2C6H3; 4-MeOC6H4; and 3-O2NC6H4. Results of tests against Staphylococcus aureus are given for V; ir and uv data are given for several compds.

L3 ANSWER 42 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **21486-57-7P 21486-59-9P 21486-61-3P**
23706-89-0P 23858-48-2P
RL: SPN (Synthetic preparation); PREP (Preparation)

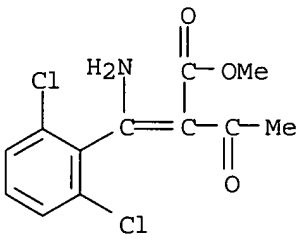
(preparation of)
RN 21486-57-7 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-, ethyl ester (8CI) (CA INDEX NAME)



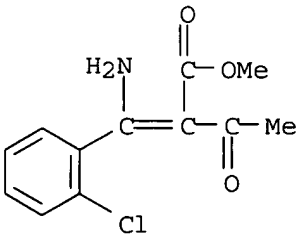
RN 21486-59-9 CAPLUS
CN Cinnamonitrile, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



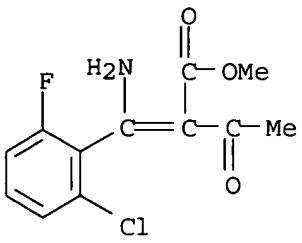
RN 21486-61-3 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-2,6-dichloro-, methyl ester (8CI) (CA INDEX NAME)



RN 23706-89-0 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-o-chloro-, methyl ester (8CI) (CA INDEX NAME)



RN 23858-48-2 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-2-chloro-6-fluoro-, methyl ester (8CI) (CA INDEX NAME)



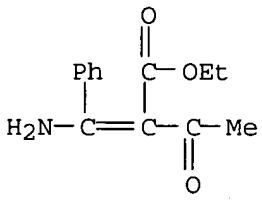
ACCESSION NUMBER: 1969:461377 CAPLUS
DOCUMENT NUMBER: 71:61377
TITLE: Antibacterial isothiazole-4-carboxylic acids
INVENTOR(S): McGregor, Donald N.; Cheney, Lee C.
PATENT ASSIGNEE(S): Bristol-Meyers Co.
SOURCE: Fr., 11 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1535809		19680809		
DE 1670248			DE	
GB 1199578			GB	
US 3498995		19700000	US	
PRIORITY APPLN. INFO.:			US	19660725

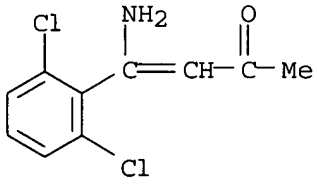
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The title compds. (I) or precursors (II), in which R1 can be hydrolyzed to a CO2H group to give I, were prepared by the action of P2S5 and an oxidant on RC(NH2):CR1COR2 (III) at 75-200°. Hydrogenolysis of 100 g. 4-carbomethoxy-3-(2,6-dichlorophenyl)-5-methylisoxazole (U.S. 2,996,501) on 50 g. Ni in 1.1 l. EtOH gave 59.6% 1-amino-2-carbomethoxy-1-(2,6-dichlorophenyl)-1-buten-3-one (IIIa), m. 155-6.5° (PhMe). Heating IIIa with P2S5 and S, iodine, air, or chloranil gave 4 - carbomethoxy - 3 - (2,6 - dichlorophenyl) - 5 - methylisothiazole (IIa). For example, 2.88 g. IIIa, 6.66 g. P2S5, and 2.45 g. chloranil in 50 ml. PhMe refluxed 15 min. gave 53% IIa, m. 81-4° (aqueous MeOH), which was saponified to the acid, m. 211-12°. The action of 300 ml. NH4OH on 50 g. 3-(2,6-dichlorophenyl)-5-methyl-4-isoxazolecarbonyl chloride in 300 ml. tetrahydrofuran at 25° 18 hrs. gave 61% 4-carbamoyl-3-(2,6-dichlorophenyl)-5-methylisoxazole (IV), m. 166° (aqueous EtOH). Dehydration of 26 g. IV by 200 ml. POCl3 and 36 ml. Et3N gave 80% 4-cyano-3-(2,6-dichlorophenyl)-5-methylisoxazole (V), m. 99-100° (aqueous Me2CHOH). Hydrogenolysis of 5 g. V in 100 ml. EtOH on 2 g. Ni gave 2.26 g. 1-amino-2-cyano-1-(2,6-dichlorophenyl)-1-buten-3-one (IIIb), m. 231-2° (n-C6H14). P2S5 (8 g.), 1.15 g. S, and 3 g. IIIb in 80 ml. PhMe refluxed 3 hrs. gave 33% 4-cyano-3-(2,6-dichlorophenyl)-5-methylisothiazole, m. 120-2° (EtOH). To 37.8 g. 2,6-Cl2C6H3CH:NOH in 200 ml. H2O at 5-10° was added 425 ml. 5.25% NaOCl. The precipitate of 2,6-dichlorobenzonitrile oxide in 200 ml. absolute EtOH was treated at 5° with 30 g. EtCOCH2CO2Et, then with 1.76 g. NaOH in 40 ml. EtOH to give 53.5% 4-carbethoxy-3-(2,6-dichlorophenyl)-5-ethylisoxazole (VI), m. 62-3° (Skellysolve B). Hydrogenolysis of 31.8 g. VI gave 83% 1-amino-2-carbethoxy-1-(2,6-dichlorophenyl)-1-penten-3-one (IIIc), m. 109.5-11.5° (Skellysolve B). IIIc (3.16 g.), 6.65 g. P2S5, and 0.96 g. S in 80 ml. PhMe gave 1.37 g. 4-carbethoxy-3-(2,6-dichlorophenyl)-5-ethylisoxazole, oil, which was hydrolyzed to 59% 3-(2,6-dichlorophenyl)-5-ethyl-4-iso-thiazolecarboxylic acid, m. 206-8° (PhMe). 6-Aminopenicillanic acid was acylated by the acid chloride of this product to give 63.5% Na 6-[3-(2,6-dichlorophenyl)-5-ethyl-4-isothiazole-carboxamido]penicillanate. Other compds. prepared were: 52 g. 3-(2-chloro-6-fluorophenyl)-5-methyl-4-isoxazolecarboxylic acid, m.

205-6° (aqueous MeOH), from 52 g. 2-chloro-6-fluorobenzaldoxime; 37 g. 4-carbomethoxy-3-(2-chloro-6-fluorophenyl)-5-methylisoxazole, m. 55-6° (cyclohexane), from 51 g. acid, via the acid chloride, 1-amino-2-carbomethoxy-1-(2-chloro-6-fluorophenyl)-1-buten-3-one, and 3-(2-chloro-6-fluorophenyl)-5-methyl-4-isothiazolecarboxylic acid, m. 199-201° (1:1 EtOH-H2O); 57.5% 1-amino-2-carbomethoxy - 1 - (2 - chlorophenyl) - 1-buten-3-one, m. 89-91° (cyclohexane), from 25.2 g. 4-carbomethoxy-3-(2-chlorophenyl)-5-methylisoxazole, and 3-(2-chlorophenyl)-5 - methyl - 4 - isothiazolecarboxylic acid, m. 187-8° (PhMe); 1-amino-2-carbethoxy-1 - phenyl - 1 - buten - 3 - one, m. 76-7° (PhMe), and 5-methyl-3-phenyl-4-isothiazolecarboxylic acid, m. 154-4.5°; and 3,5-dimethyl-4-isothiazolecarboxylic acid, sublimes 180-200°.

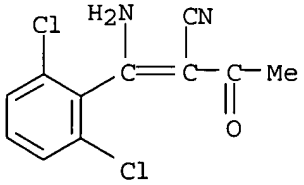
L3 ANSWER 43 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **21486-57-7P 21486-58-8P 21486-59-9P**
21486-60-2P 21486-61-3P 21486-62-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21486-57-7 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-, ethyl ester (8CI) (CA INDEX NAME)



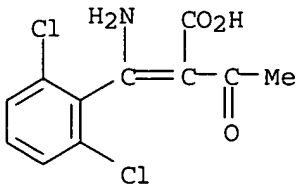
RN 21486-58-8 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(2,6-dichlorophenyl)- (8CI) (CA INDEX NAME)



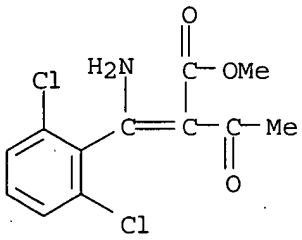
RN 21486-59-9 CAPLUS
CN Cinnamonitrile, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



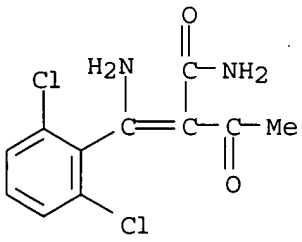
RN 21486-60-2 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



RN 21486-61-3 CAPLUS
CN Cinnamic acid, α-acetyl-β-amino-2,6-dichloro-, methyl ester (8CI) (CA INDEX NAME)



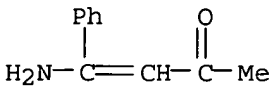
RN 21486-62-4 CAPLUS
CN Cinnamamide, α-acetyl-β-amino-2,6-dichloro- (8CI) (CA INDEX NAME)



ACCESSION NUMBER: 1969:77853 CAPLUS
DOCUMENT NUMBER: 70:77853
TITLE: Synthesis of isothiazoles. Transformation of isoxazoles into isothiazoles
AUTHOR(S): McGregor, Donald N.; Corbin, U.; Swigor, J. E.; Cheney, Lee C.
CORPORATE SOURCE: Bristol Lab. Div., Bristol-Myers Co., Syracuse, NY, USA
SOURCE: Tetrahedron (1969), 25(2), 389-95
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:77853
ABSTRACT:

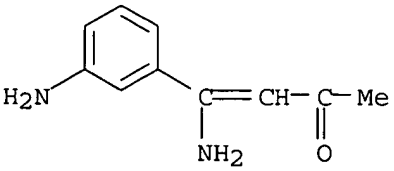
A method was devised whereby 3-(R-substituted)-4-(R1-substituted)-5-(R2-substituted)isoxazoles can be efficiently converted to 3-(R-substituted)-4-(R1-substituted)-5-(R2-substituted) isothiazoles. The isoxazole ring is opened by reduction with Raney Ni, and the resulting enamino ketone H2NCR:CR1COR2 is treated with P2S5 and chloranil to give the corresponding isothiazole derivative Thus, by taking advantage of the relatively numerous and reliable routes available for the preparation of variously substituted isoxazoles, it is possible to obtain readily many isothiazole derivs. which were previously available only with great difficulty.

L3 ANSWER 44 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**
RL: PRP (Properties)
(conformation of, calcn. of)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1967:24254 CAPLUS
DOCUMENT NUMBER: 66:24254
TITLE: Chemical exchange processes [examined] by means of nuclear magnetic resonance
AUTHOR(S): Bhar, B. N.; Daehne, Siegfried; Klose, Gotthard; Ranft, Johannes
SOURCE: Wissenschaftliche Zeitschrift der Humboldt-Universitaet zu Berlin, Mathematisch-Naturwissenschaftliche Reihe (1965), 14(4), 871-5
CODEN: WZHMAE; ISSN: 0522-9863
DOCUMENT TYPE: Journal
LANGUAGE: German
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Exchange of the type shown was studied for 2,5-bis(dimethylamino)benzoquinone (I) and 2,5-bis(1-pyrrolidinyl)benzoquinone. For I: ΔE = 18.5 ± 4 kcal./mole, k0 = 1.1 + 1019, and for II: ΔE = 10.0 ± 3.0 kcal./mole, k0 = 1.3 + 109 were obtained. The N.M.R. spectra for MeC(NH2):CHCOMe indicate a barrier of 6 ± 3 kcal./mole for internal rotation about the C-N bond. A study of the spectrum of 2-pyridylmethyl Ph ketone indicated that exchange between several forms takes place, probably involving structures such as III and IV.

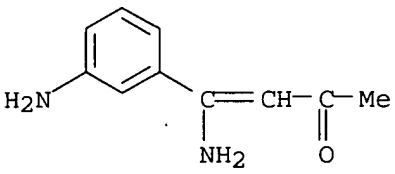
L3 ANSWER 45 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **91842-83-0**, 3-Buten-2-one, 4-amino-4-(m-aminophenyl)-
(preparation of)
RN 91842-83-0 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(m-aminophenyl)- (7CI) (CA INDEX NAME)



ACCESSION NUMBER: 1964:30882 CAPLUS
DOCUMENT NUMBER: 60:30882
ORIGINAL REFERENCE NO.: 60:5475d-g
TITLE: Derivatives of 6-aminopenicillanic acid. VII. Further 3,5-disubstituted isoxazole-4-carboxylic acid derivatives
AUTHOR(S): Doyle, F. P.; Hanson, J. C.; Long, A. A. W.; Nayler, J. H. C.
SOURCE: Journal of the Chemical Society, Abstracts (1963), (Dec.), 5845-54
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal

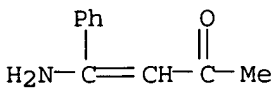
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:30882
ABSTRACT:
Further 3,5-disubstituted isoxazole-4-carboxylic acids were prepared as intermediates for the synthesis of penicillins, many of which resisted inactivation by penicillinase.

L3 ANSWER 46 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **91842-83-0**, 3-Buten-2-one, 4-amino-4-(m-aminophenyl)-
(preparation of)
RN 91842-83-0 CAPLUS
CN 3-Buten-2-one, 4-amino-4-(m-aminophenyl)- (7CI) (CA INDEX NAME)



ACCESSION NUMBER: 1964:30881 CAPLUS
DOCUMENT NUMBER: 60:30881
ORIGINAL REFERENCE NO.: 60:5475c-d
TITLE: Derivatives of 6-aminopenicillanic acid. VI. Penicillins from 3- and 5-phenylisoxazole-4-carboxylic acids and their alkyl and halogen derivatives
AUTHOR(S): Doyle, F. P.; Hanson, J. C.; Long, A. A. W.; Nayler, J. H. C.; Stove, E. R.
SOURCE: Journal of the Chemical Society, Abstracts (1963), (Dec.), 5838-45
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
cf. CA 58, 6816f. Condensation of benzohydroxamoyl chloride or its Me or halogen derivs. with the Na derivs. of acylacetic esters gave a series of 3-arylisoxazole-4-carboxylic acids.. The 5-aryl analogs were prepd, from α-alkanoyl-α-aroylacetic esters and NH2OH. The 3- and 5-aryl acids were differentiated by means of their ultraviolet spectra. Reaction of the isoxazole acid chlorides with 6-aminopenicillanic acid gave isoxazolylpenicillins (I) with useful antibacterial activity.

L3 ANSWER 47 OF 47 CAPLUS COPYRIGHT 2005 ACS on STN
IT **14088-41-6**, 3-Buten-2-one, 4-amino-4-phenyl-
(stereoisomers)
RN 14088-41-6 CAPLUS
CN 3-Buten-2-one, 4-amino-4-phenyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1955:4657 CAPLUS
DOCUMENT NUMBER: 49:4657
ORIGINAL REFERENCE NO.: 49:942i,943a-h
TITLE: Structure and Grignard reaction of 3-aminocrotononitrile

AUTHOR(S): Conn, Jasper J.; Taurins, Alfred
CORPORATE SOURCE: McGill Univ., Montreal, Can.
SOURCE: Canadian Journal of Chemistry (1953), 31, 1211-22
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 49:4657
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The object of this work is to study the properties of MeC(NH2):CHCN (I) in order to elucidate the nature of the high- (III) and low-melting (IV) forms and to prepare β-amino ketones by the action of Grignard reagents on I. A new mechanism for the formation of I, involving free-radical intermediates, is proposed. The preparation of the 2 modifications of I involves decomposition of the Na
salt of I at different temps. IV is obtained if the salt is decomposed at 30° whereas III is prepared with ice-cold H2O. In both cases I is extracted with Et2O and recrystd. from C6H6. Ultraviolet absorption spectra for IV: λmax.EtOH 258 mμ (ε 13600) and λmax.MeCN 254.5 mμ (ε 12430). For III: λmax.EtOH 256 mμ (ε 14700) and λmax.MeCN 254.5 mμ (ε 13650). Thus III and IV have identical electronic configurations in polar solvents and hence the existence of tautomeric forms of I are excluded. The spectra are in accordance with the enamine structure of I, which can exist as a resonance hybrid of 3 resonating structures. A determination of the heats of solution of III and IV shows identical values, hence it is safe to assume that the heats of melting of III and IV will be of the same order of magnitude and are almost identical. This conclusion serves to confirm the enamine structure of I. The existence of polymorphic modifications of I is excluded on the basis of its thermochem. behavior. It is proposed that these modifications are cis and trans isomers, IV being the cis form, III the trans form. In IV the NH2 and CN groups are in adjacent positions and can form an internal H bond (V) which makes the cis more stable than the trans isomer. I (10 g.) in 100 ml. Et2O refluxed with 0.5 mole PhMgBr in 300 ml. Et2O gives 5 g. (20%) H2NCPh:CHAc (VI), bl 70-80°; 2,4-dinitrophenylhydrazone, orange needles, m. 241-2°. VI (0.5 g.), 0.5 g. NH2OH.HCl, and 2 g. KOH in 5 ml. H2O refluxed 2 hrs. give 3-methyl-5-phenylisoxazole (VII), white needles from EtOH, m. 67°. The formation of VII is proof of the structure of VI. BzCH2Ac (VIII), m. 60-1°, is obtained in 5% yield if, after the decomposition of the Grignard complex and extraction with Et2O, the alkaline aqueous solution is neutralized with HCl and
cooled. VIII is obtained in 10% yield if the Et2O solution of the decomposed Grignard complex is repeatedly extracted with saturated NaHCO3 solution and the bicarbonate solution acidified with HCl. It is evident that VIII is formed by hydrolysis of VI. VIII with NH2OH.HCl yields VII. I (10 g.) and 0.5 mole 1-C10H7MgBr similarly give 6.5 g. (25.2%) 1-C10H7C(NH2):CHAc (IX), bl 130-5°; 2,4-dinitrophenylhydrazone, fine orange needles, m. 216-17°; semicarbazone, white plates, m. 213-14°. IX with NH2OH.HCl gives 3-methyl-5-(1-naphthyl)isoxazole, white plates, m. 140-1°. The Et2O extract of the decomposed Grignard complex extracted with NaHCO3 and neutralized with HCl gives 1.5 g. (5.8%) 1-C10H7COCH2Ac (X), fine prisms, m. 107-8°. I and o-MeC6H4MgBr (XI) give 11% o-MeC6H4C(NH2):CHAc (XII), yellow oil, b4 40-50°; 2,4-dinitrophenylhydrazone, orange needles, m. 162-3°. I and p-MeC6H4MgBr give 11-15% p-MeC6H4C(NH2):CHAc (XIII), yellow oil, b4 30-40°; 2,4-dinitrophenylhydrazone, fine red needles from C6H6, m. 259-60°. I and PhCH2MgBr give 16% PhC(NH2):CHAc (XIV), yellow oil, bl 70-5° (2,4-dinitrophenylhydrazone, orange needles, m. 146-7°). As further proof of the position of the C:O group in VI, 19.2 g. Me(PhNH)C:CHCN (XV) treated 48 hrs. with 0.75 mole PhMgBr in 400 ml. Et2O gives 6.5 g. (12%) H2NCPh:CHC(:NPh)Me (XVI), yellow crystals, m. 85-6°. XVI on acid hydrolysis with 75% H2SO4 1 hr. at 150-60° gives VI, identified as the 2,4-dinitrophenylhydrazone. The reaction of β-amino nitriles with Grignard reagents is extended to include H2NCEt:CMeCN (XVII). XVII (20.7 g.) and 0.6 mole PhMgBr in 400 ml. Et2O give

5.2 g. (15%) H2NCPh:CMeCOEt, light oil, b8 80-90°; 2,4-dinitrophenylhydrazone, bright orange needles, m. 230-1°.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	251.14	412.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-36.50	-36.50

STN INTERNATIONAL LOGOFF AT 13:42:09 ON 26 JUN 2005